M.Phil/Ph.D Physical Chemistry

CHM-776 **Nanostructures and Nanomaterials** **3(3-0)**

Learning Objectives/ Motives:

The course is designed to familiarize the students from the basic to advance trends in the field of nanoscience. No course is offered by the section of Physical Chemistry in this important area of current utility.

Proposed Contents

Introduction to nanoscience, nanomaterials and nanotechnology. Synthesis of Nanomaterials.

(Physical Methods), Mechanical Methods, Chemical Methods, Analysis Techniques for nanomaterials; Optical Microscopy, Electron Microscopy, Scanning Electron Microscopy, Transmission Electron Microscope (TEM), Atomic Force Microscopy, Diffraction Techniques, X-Ray Diffraction (XRD), Fourier Transform Infra Red Spectrometry, Mechanical Measurements. Types of Nanomaterials and Their Properties Nanoelectronics, Carbon Nanomaterials, Applications of nanotechnology, Nanotechnology and Environment.

Recommended Books

1. Misra, P. Applied Spectroscopy and the Science of Nanomaterials, 2015. Springer Singapore
   Heidelberg New York Dordrecht London
2. Br´echignac, C., Houdy, P., Lahmani, M. 2007, Nanomaterials and Nanochemistry, Springer Berlin Heidelberg New York
3. Charles P. Poole, Jr. and Frank J. Owens, Introduction to Nanotechnology. John Wiley &
   Sons, Inc., Hoboken, New Jersey, 2014.
4. Sulabha K. Kulkarni, Nanotechnology: Principles and Practices, 2015, Springer Cham Heidelberg New York Dordrecht London
5. Kalarikkal, N., Thomas, S., Koshym O. 2018, Nanomaterials; Physical, Chemical, and Biological Applications. CRC Press, Taylor & Francis Group.
6. Khan, Z.H. 2018, Nanomaterials and their applications. Springer, Singore.
7. Hosseinkhani, H., 2019. Nanomaterials in advanced Medicines. Wiley-VC.
8. Sengupta, A., Sarkar, C.K. 2015. Introduction to Nano, Basics to Nanoscience and Nanotechnology. Springer.
9. Sattler, D. K.2014, Handbook of Nanophysics, Nanoelectronics and Nanophotonics. . CRC Press, Taylor & Francis Group.
10. Johal S. M., Johnson L.E. 2018, Understanding Nanomaterials. 2nd Ed. CRC Press, Taylor & Francis Group.

11. Azamal, H. Muhammad, I. 2019, Nanomaterials and Plant Potential, Springer Nature Switzerland AG.

CHM-777 **Advanced Functional Materials** **3(3-0)**

Learning Objectives/ Motives:

It is an advance level course of material chemistry, with the aim to enlighten the students about the recent trends in modern materials. A basic course is offered by the section of Physical chemistry on this topic in BS/MSC Specialization.

Contents

Introduction and applications of; thermal expansion materials, Shape memory alloys, Electroactive Smart Materials, Photoadhesive Smart Materials, Photochromic Materials, Thermochromic and Thermotropic Smart Materials, Light Emitting Smart Materials, Photoluminescent Smart Materials, Electroluminescent Smart Materials, Thermoelectric Smart Materials, Electroluminescent Smart Materials, Electricity Generating Smart Materials, Piezoelectric Smart Materials, Energy Storage Smart Materials, Matter Exchanging Smart Materials. Bio-based polymeric materials, biomaterials, biomedical applications of smart biomaterials

Recommended Books

1. Aguilar, M.R and Román, J.S. Smart Polymers and their Applications, 2014, Woodhead Publishing Limited.
2. Hey-Hawkins, E and Hissler, M. Smart Inorganic Polymers Synthesis, Properties, and Emerging Applications in Materials and Life Sciences, 2019. Wiley-VCH Verlag GmbH & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany.
3. Galaev , I. Mattiasson, B. SMART POLYMERS Applications in Biotechnology and Biomedicine, Second Edition, 2008, CRC Press Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742.
4. Ponnamma, D. Sadasivuni, K.K. Cabibihan, J. J. Al-Maadeed, M.A. Smart Polymer Nanocomposites Energy Harvesting, Self-Healing and Shape Memory Applications, 2017, Springer International Publishing AG Gewerbestrasse 11, 6330 Cham, Switzerland.
5. Miyazzaki, S., Fu, Y.Q., Haung, W.M., Thin film shape memory alloys, Fundamentals and Device Applications. 2009, Cambridge University Press. New York. USA.
6. Kalia, S., Averous, L., Biodegradable and biobased Polymers for Environment and Biomedical Applications. 2016, Scrivener Publishing, Co published by John Wiley & Son, Inc. Hoboken, New Jersey, and ScrivenerPublishing LLC, Salem, Massachusetts. Published Simultaneously in Canada.

7. Fleischer, A.S. Thermal Energy storage using phase change Materials. Fundamentals and Applications. 2015. Springer. USA.
8. Makhlouf, A.S.H.Hand book of smart coatings for materials protection 2014. Woodhead Publishing.
9. Colin, T. Introduction to Materials for Advanced Energy Systems, Springer Nature Switzerland AG, 2019.

CHM-778 Renewable Resources – Chemistry and Technology 3(3-0)

Learning Objectives/ Motives:

Students after passing this course should be able to make interpretation about the energy sources, integrate knowledge and physical techniques to solve important natural resource management problems with use of renewable energy resources. They should be able to work for the future sustainability of natural resources by using renewable technologies. They will be able to comprehend the energy and energy types like make interpretation about the solar energy, geothermal energy, solar energy collectors, wind energy and the hydrogen energy.

Course contents: Introduction to global primary energy consumption and reversible energy resources; Reason to use renewable energy sources; Solar energy; Solar photovoltaic devices; Solar cells; Thermal power plants; Biomass (solid, liquid and gaseous biofuels) energy; Environmental impact of biomass energy; Hydrogen as clean fuel of the future; Solar cells and other renewable resources (wind, geothermal, hydroelectric power and tide power).

Reference Books:

1) "Advances in Renewable Energies and Power Technologies Volume 1: Solar and Wind Energies" Edited by Imene Yahyaoui, 2018 Elsevier Inc. Radarweg 29, PO Box 211, 1000 AE Amsterdam, Netherlands.
2) "Renewable-based technology: sustainability assessment" by Jo Dewulf, Herman Van Langenhove, 2006, Wiley.
3) "Chromatography for sustainable polymer materials: degradable and recyclable" by Lina Burman, Ann-Christine Albertson, Minna Hakkarainer, 2008, Springer-Verlag Berlin Heidelberg.
4) "Bioprocessing for value added products from renewable resources: New technologies and applications" by Shang-Tian yang, 2007, Elsevier Science.
5) Renewable resources and renewable energy: A global challenge" by Paolo Fornasiero, Mauro Graziani, 2006. CRC press.
6) "Monomers, polymers and composite for renewable resources" by Mohammad Naceur Belgacem, Alessandro Gandini, 2008, Elsevier.

7) "Energy Efficiency and renewable Energy" Edited by D. Yogi Goswami Frank kreith, Hand book, Second Edition, 2016 by Taylor & Francis Group, LLC.
8) " Fundamental of renewable energy processes" by Aldo V. Da Rosa, 2005, Elsevier.
9) "Kicking the carbon habit: Global warming and the case for renewable and nuclear energy" by William Sweet, 2006, Columbia University Press.
10) "Nanotechnology for electronics, photonics and renewable energy" by Paolo Lugli, Simone Locci, Christoph Erlen, Anatoli Korkin, Predrag S. Kristic, jark C. Wells, 2010, Springer-Verlag new York.
11) "The nanoscience and technology of renewable biomaterials" by Prof. Lucian Lucia, Orlando Rojas, 2009, Wiley-Blackwell.
12) "Surfactants from renewable resources" by Mikeal Kjellin, Inge Gard Johnsson, 2010, Wiley.
13) "Solar hydrogen generation towards a renewable energy future" by Krishnan Rajeshwar, Robert mcconnell, Staurt Licht, 2008, Springer.

CHM-779 PHOTOVOLTAIC MATERIALS AND SOLAR CELLS 3(3-0)

Learning Objectives/ Motives:

This course will demonstrate the basic understanding of the fundamentals of photovoltaic systems and solar energy.Students will learn about the chemistry of different photovoltaic technologies that are used to harness the power of solar energy along with the future perspectives of different solar cells materials.Previously, this course was not taught in the Department of Chemistry GCUF, which is a hot topic now a days in the field of renewable energy resources utilization.

Course contents: Renewable energy resources with emphasis on solar energy and solar spectrum. Brief history, principle and working of photovoltaic cells. J-V characteristics, short circuit current, open circuit voltage and fill factor. Direct and indirect band gap materials, electronic states, doping and impuritiesin semiconductors. P-N junction, metal-semiconductor junction, semiconductor-semiconductor junction and electrochemical junctions.Different generations of photovoltaic cells, silicon based solar cells, thin film solar cells, organic solar cells, quantum dot solar cells, concept and working principle of dye-sensitized solar cells along with hybrid perovskite solar cells and bulk heterojunction solar cells. Drift and diffusion equations for current flow.Charge carriergeneration and recombinationprocesses.Shockley-Queisser limitand future of photovoltaics.

Recommended Books

1. R. J. Komp, Practical Photovoltaics: Electricity from Solar Cells, Aatec Publications, Michigan USA, 2001.
2. M.A. Green, Third Generation Photovoltaics: Advanced Solar Energy Conversion, Springer, New York, 2007.

3. A. H. M. Smets, K. Jager, O. Isabella, R.A.C.M.M. Swaaij, M. Zeman,Solar Energy: The Physics and Engineering of Photovoltaic conversion, Technologies and Systems, Cambridge, England,2006.
4. K. Jager, O. Isabella,A. H. M. Smets,R.A.C.M.M.Swaaij, M. Zeman,Solar Energy: Fundamentals, Technology, and Systems, Delft University of Technology,Netherlands, 2014.
5. K. Mertens, G. Roth, Photovoltaics Fundamentals, Technology and Practice, Wiley, United Kingdom, 2014.
6.A. Goetzberger, V.U. Hoffmann, Photovoltaic Solar Energy Generation, Springer, USA, 2005.
7. J. Bisquert, The Physics of Solar Cells Perovskites, Organics, and Photovoltaic Fundamentals, Taylor & Francis Group, LLC. 2018.
8. A. A. Ojo , W. M. Cranton, I. M. Dharmadasa, Next Generation Multilayer Graded Bandgap Solar Cells, Springer International Publishing AG, part of Springer Nature, 2019.

CHM-780 Polymer Mechanochemistry 3(3-0)

Basis of the theory of local character of deformation, The local character of polymer fracture, Deformation and fracture – interconnected processes, Mechanochemical mechanism of polymer deformation, Mechanochemistry of polymer deformation under creep conditions, Chemical stress relaxation, Mechanochemical reactions at fracture surfaces, Mechanochemical mechanism of fracture, Factors that influence the mechanodegradation process, Structural factors, Characteristics of supramolecular–morphological structure Mechanochemical reactions at fracture surfaces, Modification of the structure-properties relationship by polymer degradation and fracture.

Recommended Books

1. Macromolecular Mechanochemistry, Polymer Mechanochemistry, Vol 1, Part 1, 2006, Cleopatra. V. Oprea., Florin, D.Cambridge International Science Publishing.
2. Ali. S. Argon, The Physics of deformation and fracture of polymers, 2013. Cambridge University Press, New York
3. Nestor, P. Fracture Mechanics, 2004, Kluwer Academic Publishers

CHM-781 Physical Chemistry of High Polymers 3(3-0)

Molecular forces and chemical bonding in polymers, configuration and conformation of polymer chains, theories of polymer solutions; phase separation and fractionation, plasticization, molecular size measurement, spectroscopic analysis, thermal analysis, morphology and order in crystalline polymers, polymer reheology, electrical and magnetic properties of polymers.

Recommended Books:

1. Flory, “Principle of Polymer Chemistry” Cornell University press, New York,

USA (1953).
2. Fried J. R. “Polymer Science and Technology”2nd Ed., Prenitce Hall, USA (1995).
3. Young, R.J. “Introduction to Polymers”. 2nd Ed., Chapman and Hall Ltd, UK (1981).

CHM-782 Complex Extension of Quantum Chemistry 3(3-0)

Revision of basic quantum (Historic background, Uncertainty principle, Time-dependent/Time-independent Schrödinger equation, Probability, complex number, Particle in one dimensional box, Tunneling, Operators) Particle in three dimensional box, Requirements of an acceptable wave function, The Harmonic oscillator (one-dimensional harmonic oscillator, Vibration of molecules, Numerical solution of one-dimensional Schrödinger equation), Angular momentum, The Hydrogen atom , Theorems of quantum mechanics (Hermitian operator, Parity, Matrices), The Variation Method (Variation theorem, Determinants, Linear variation methods), Perturbation Theory (Non-degenerate perturbation theory, Perturbation treatment of the Helium atom ground state, perturbation theory for a degenerate energy level).

Recommended Books:

1. I. N. Levine. “Quantum Chemistry, fifth edition” Prentice-Hall, Inc. Upper Saddle River, New Jersey, USA (1991).
2. J. P. Lowe, K. A. Peterson. "Quantum Chemistry” 3rd Ed, Elsevier Academic Press, Netherland (2006).
3. P. A. Cox, "Introduction to Quantum Theory and Atomic Structure", Oxford University Press, UK (2002).
4. P. W. Atkins. "Molecular Quantum Mechanics" Oxford Univ. Press, Oxford, England (1983).
5. M. Muller. "Fundamentals of Quantum Chemistry", Kluwer Academic Publishers, Boston, USA (2001).

CHM-783 Electrode Processes 3(3-0)

Theories of electron transfer reactions, electron transfer process, electroanalytical techniques, methods for studying homogeneous and heterogeneous electron transfer reactions. semiconductor electrochemistry. Industrial electrochemistry. Eletro-chemical energy conversion systems.

Recommended Books:

1. J. Albert, “Electrode Kinetics” Clarendon, Oxford, UK (1975).
2. A. Bard, L. R. Faukner, “Electrochemical Methods, Fundamentals and Application” 2nd Ed., John Wiley and Sons, New York, USA (2001).
3. M. Mohammad, M. Amjad, “Principles of Electrode Kinetics” Rooha Printers, Lahore, Pakistan (2001).

CHM-784 Magnetic Spin Dynamics 3(3-0)

Revision of basic magnetic spin dynamics (Classical, quantum and spin angular momentum, nuclear spin and nuclear Zeeman splitting, quadruple nuclei with integer and half integer spin, magnetism, macroscopic and microscopic magnetism, simple pulse sequence, in homogeneous broadening, chemical shift, heteronuclear decoupling). The NMR spectrometer(the magnet, transmitter section, the duplexer, the probe, the receiver section, overview of radiofrequency section, Pulse gradient section), Fourier transform NMR (heteronuclear experiments, Arrayed experiments, two dimensional spectroscopy, three dimensional spectroscopy), mathematical techniques, Quantum mechanics (functions, operators, eigen functions, eigen values, eigen vectors, diagonalization, exponential operators)

Recommended Books:

1. M. H. Levitt. "Spin Dynamics, Basics of Nuclear Magnetic Resonance" John Wiley and Sons, New York, USA (2008).
2. N. E. Jacobsen. "NMR spectroscopy explained" John Wiley and Sons. New York, USA (2007).
3. R. S. Macomber. "A complete introduction to modern NMR Spectroscopy" John Wiley and Sons, New York, USA (1998).

CHM-785 Molecular Spectroscopy 3(3-0)

Microwave, infrared and Raman Spectroscopy. Normal coordinate analysis. Electronic spectra of diatomic and simple polyatomic molecules. Molecular symmetry, group theory and applications in chemistry. Applications of spectroscopy in structural chemistry

Recommended Books:

1. C. N. Banwell, “Fundamentals of Molecular Spectroscopy” 3rd Ed., Tata McGraw Hill, USA (1992).
1. G. M. Barrow, “Introduction to Molecular Spectroscopy,” 2nd Ed., McGraw-Hill, New York, USA (1962).
3. J. D. Graybal, “Molecular Spectroscopy,” McGraw-Hill, New York, USA (1988).

CHM-786 Photochemistry 3(3-0)

Principle of photochemistry. Sources of radiation, actinometry (both physical and chemical), primary and secondary photochemical processes, quantum yields, experimental techniques, photolytic studies of aqueous and non-aqueous systems, effects of radiation on solids. Kinetics, mechanism, energetics of photochemical reactions.

Recommended Books:

1. D. Neckers, G.N.V.B, Nau, "Advances in Photochemistry" Volume 27, John Wiley & Sons, New York, USA (2002).
2. P. Suppan, "Chemistry and Light" The Royal Society of Chemistry, London, UK (1994).
3. R. P. Wayne, "Principles and Applications of Photochemistry, Oxford University Press, UK (1998).

CHM-787 Solution Chemistry 3(3-0)

Physicochemical characteristics of solvents. Solute-solvent interaction, salvation of ions, preferential salvation. Thermodynamic properties of solute in bare solvents and mixed solvents. Transport properties of solutions, concept of association constant of ions in solution. Study of solute-solvent-solute interactions by spectroscopic techniques.

Recommended Books:

1. R. A. Alberty, J. S. Robert, G. B. Moungi, "Physical Chemistry". 4th Ed, John Wiley and Sons, New York, USA (2004).
2. D. W. Ball, "Physical Chemistry" 1st Ed., Brooks/Cole Co. USA (2003).
3. Smith, E. Brian, "Basic Chemical Thermodynamics" 5th Ed, Imperial College Press, UK (2004).
4. B. R. Stephen, S. A. Rice, J. Ross, "Physical Chemistry" 2nd Ed, Oxford University Press, UK (2000).
5. W. Jurg, "Basic Chemical Thermodynamics" 4th Ed., W. A. Benjamin (1969).
6. R. G. Mortimer. "Physical Chemistry" 3rd Ed, Elsevier Academic Press, UK (2008).

CHM-788 Colloids and Surfactants 3(3-0)

Liquid interfaces, surface tension and adsorption from solution, insoluble surface monolayer (Langmuir-Blodgett films). Surfactant, detergency, organized molecular assemblies (micelles, vescicles and membranes). Micro and macroemulsions. Colloidal dispersions, coagulation and flocculation. Optical properties of colloids.

Recommended Books:

1. M. J. Rosen, "Surfactants and Interfacial Phenomena" Marcel Dekker Inc., New York, USA (1989).
2. P. C. Hiemenz, R. Gopalan, "Principles of Colloid and Surface Chemistry" 3rd Edition, Marcel Dekker Inc., New York, USA, (1997).
3. D. F. Evans, "The Colloidal Domain", VCH, Weinheim, Germany (1994).

CHM-789 Theoretical and Computational Chemistry 3(3-0)

Molecular orbital calculations. Essential concepts, semiempirical and Ab-initio methods. Reactivity. Configuration interaction method. Potential energy surfaces. Quantitative structura-activity relationship (QSAR). Molecular mechanics. Energy minimization force field parameterization and conformational analysis. Computer programming and three dimensional graphics using standard packages.

Recommended Books:

1 C. J. Crammer, "Essentials of Computational Chemistry" John Wiley and sons, New York, USA (2002).
2 F. Jenson, "Introduction to Computational Chemistry" Wiley, USA (2000).
3 K. B. Lipkowitz, D. B. Boyd, "Reviews in Computational Chemistry ", VCH, New York, USA (1991).

CHM-790 Advanced Composite Materials 3(3-0)

Definitions and classification, natural composites. Property enhancement by reinforcement and orientation, matrix interface, synthetic fibers, properties and processing of composites with metallic, ceramic and polymeric matrices, interface reactions, mechanical and thermal properties of composite materials, stress relaxation and creep studies, dynamical mechanical properties, toughening mechanism and mechanical failure in polymeric composites.

Recommended Books:

1. F. L. Mathews, R. D. Crawlings, "Composite Materials: Engineering and Science, Chapman and Hall, UK (1994).
2. R. E. Shalin, "Polymer Matrix composites", Chapman and Hall, UK (1995).
3. R. S. Scifullon, "Physical Chemistry of Inorganic Polymers and Composite materials", Ellis Harwood, UK (1992).

CHM- 791 Heterogeneous Catalysis 3(3-0)

Introduction to catalysis, Classification of catalytic systems, classification of solid catalysts, adsorption of molecules at the solid surfaces, adsorption isotherms, surface area and porosity, adsorbed states of molecules on metal surfaces, potential energy curves for adsorption, descriptive chemistry of chemisorptions on metals, quantitative aspect of chemisorptions on metals, sorption on oxide surfaces, the band theory of solids, adsorption on insulator oxides, kinetics of heterogeneous reactions, mass transport limitation of catalyzed reactions. Catalysis in energy conversion and in the production of hydrocarbon feed stock, Oxidation catalysis: The Petrochemical Industry, Catalysis in the inorganic chemical industry, Catalysis in Atmospheric Pollution Control

Recommended books:

1. Bowker, M. "Basics and Application of Heterogeneous Catalysis" Oxford, 1998.
2. Gates, B.C. Catalytic Chemistry, John Wiley, 1992.
3. Bond, G.C. Heterogeneous Catalysis: Principals and applications, Oxford, 1987.
4. Boudart, M. and Mariadassou, G.D. "Kinetics of Heterogeneous Catalytic Reactions" Princeton, 1984.

CHM-792 Modern Aspects of Chemical Kinetics 3(3-0)

Chemical Kinetics, Development and modern use of chemical kinetics. Potential energy surfaces, statistical and quantum mechanical approaches for the study of unimolecular decomposition rate. Transition state theory and microscopic reversibility. Applications of transition state theory. Effect of temperature, Pressure, volume, Solvent and salt on rate of a reaction and determination of their respective kinetic expression. kinetic isotopic effects. Composite rate constants, isokinetic relationship. Catalysis and application of kinetics study for the production of enzymes. Kinetics of photochemical reactions. Kinetics of very fast reactions. Application of kinetics in modern industries. Kinetics study of drug (in-vivo and in-vitro). Importance of kinetics for military applications

Books Recommended:

1. R. Alberty, "Physical Chemistry" 17th Ed, John Wiley and Sons, New York, USA (1987).
2. P. W. Atkins, "Physical Chemistry" 6th Ed, W. H. Freeman and co. New York, USA (1998).
3. K. J. Laidler, "The World of Physical Chemistry*"* 1st Ed., Oxford University Press, UK (1993).
4. K. J. Laidler, H. M. John, C. S. Bryan, "Physical Chemistry" 4th Ed., Houghton Mifflin Publishing Company Inc., USA (2003).
5. M. G. Barrow, "Physical Chemistry" 5th Ed., Mc Graw Hill, USA (1992).

CHM-793 Environmental Chemistry and Energy Conversions 3(3-0)

Environmental Chemistry: global perspective, Earth atmosphere, study of reactions in regions of atmosphere. Chemistry of ozone formation and decomposition, ozone depletion. Air pollution, acidifying agents in rain, adverse effects and prevention. Chemistry of urban atmosphere. Indoor air pollution. Water pollution and chemistry of wastewater treatment methods (Physical, chemical and biological). Solid waste and Nuclear waste management. Nomenclature & Chemistry of CFC's. Experimental techniques for environmental monitoring. Renewable energy resources with reference to green fuels. HAARP technology.

Books Recommended:

1. G. W. Vanloon, S. J. Duffy, "Environmental Chemistry", A Global perspective, Oxford University press INC., UK (2000).
2. S. E. Manahan, "Environmental Science and Technology" Lewis Publishers, New York, USA (1997).
3. J. W. Moore, E. A. Moore, "Environmental Chemistry", Academic Press Inc., New York, USA (1990).
4. A. D. Kumar, "Environmental Chemistry", 2nd Ed, Wiley Eastern Ltd. India (1993).

CHM-794 Surface Chemistry 3(3-0)

Solid-liquid interface. Adsorption from solutions. Gibbs absorption isotherm. Solid-gas interface, adsorption isotherms. Diffusion limitations and compensation effect. Catalysis, homogeneous and heterogeneous catalysis. Catalytic activity geometric factor in catalysis, supported metal catalysts, catalytic reactors, catalytic preparation techniques. Applied catalysis in steam reforming reaction, methanation reaction, Fisher-Tropsch synthesis, ammonia synthesis processes.

Recommended Books:

1. G. C. Bond, "Heterogeneous Catalysis" 2nd Ed. Clarendon Press. Oxford, UK (1987).
2. S. G. Gregg, K. S. W. Sing, "Adsorption, Surface area and Porosity" 2nd Edition, Academic Press, London, UK (1982).
3. M. J. Jaycock, G. D. Parfitt, "Chemistry of Interfaces", Ellis Horwood Ltd. Chichester, UK (1981).

CHM-795 Solid State and Semiconductors 3(3-0)

Solid state. Metal conductors. Band theory. Semiconductors. Insulators. Work function. Electrochemical Potential and Fermi levels. Superconductivity Recent theories, preparation and characterization of superconducting ceramics and their electrical and magnetic properties.

Books Recommended:

1. W. D. Callister, "Material Science and Engineering" 6th Ed., John Wiley and Sons, New York, USA (2003).
2. A. R. West, "Solid State Chemistry" 2nd Ed, John Wiley & Sons, USA (2002).
3. J. R. Christman, "Fundamentals of Solid State Physics" John Wiley & Sons, New York, USA (2003).

CHM-796 Thermodynamics and Statistical Mechanics 3(3-0)

Revision of basic thermodynamics and statistical mechanics (Boltzmann distribution law

and statistical thermodynamics, nature and aim of statistical mechanics, the partition function and statistical thermodynamics, the ideal gas, translational, rotational and vibrational partition function, law of equipartition of energies, chemical equilibrium in ideal gas mixtures), thermodynamic functions, Ideal harmonic solids and black body radiations (Ideal harmonic crystals, Rayleigh-Jeans law, Debye theory of the heat capacity of solids, blackbody radiations), the third law (Nernst heat theorm in thermodynamics, third law in statistical mechanics), The non ideal gas(Virial coefficients, intermolecular forces, second virial coefficient from statistical mechanics long range forces), the liquid state (structure of liquids, equation of liquid state, computer simulations), Quantum ideal gases (Bose-Einstein and FermiDirac statistics, grand canonical partition function).

Books Recommended:

1. M. R. Wright, "An Introduction to Chemical Kinetics" John Wiley and Sons, New York, USA (2004).
2. R. Alberty, "Physical Chemistry" 17th Ed., John Wiley and Sons, New York, USA (1987).
3. P. W. Atkins, "Physical Chemistry" 6th Ed, W. H. Freeman and co. New York, USA (1998).

CHM-797 Environmental applications of High Energy radiations 3(3-0)

Introduction and development of Radiation chemistry. Radiation sources, Particle accelerators. Interaction of ionizing radiation with matter. Linear energy transfer. Dosimetry terms and units, Primary and Secondary Dosimetry, Calculation of absorbed dose in samples. Chemistry of scavenger, Ion scavenger, radical scavenger. Radiolysis of water (Vapour, Ice and Liquid water). Treatment of liquid effluents, Flu gas and sludge. by ionizing radiation. Radiolytic degradation of model organic compounds.

Books recommended:

1. J. W.T. Spinks and R. J. Wood, An Introduction to Radiation Chemistry Third edition, (1990), John Wiley & Sons, INC New York.
2. G. R. Choppin, J Rayberg " Nuclear Chemistry, Theory and Application". 1st edition, Pergaman Press, Oxford, USA (1998)
3. F. Aziz, M. A. J. Rodgers, Radiation Chemistry Principle and Application". VCH Publisher, Inc, (1987).

CHM-798 Instrumental Physical Chemistry 3(3-0)

Magnetic resonance spectroscopy: Introduction, magnetic resonance imaging(MRI), nuclear magnetic resonance in solid state. Diffraction methods: introduction, single

crystal, x-ray diffraction of small molecules and macromolecules including natural systems; Powder x-ray diffraction of small molecules and macromolecules. Electron microscopy: introduction; scanning electron microscopy(SEM), transmission electron microscopy(TEM). Fluorescence techniques: steady state fluorescence, time resolved fluorescence.

Books Recommended:

1 E. M. Haacke, R. W. Brown, M. L. Thompson, Venkatesan "Magnetic Resonance Imaging: Physical Priciples and Sequence Design" John Wiley and Sons, New York, USA (1999).
2 M. J. Duer, "Introduction to Solid State NMR Spectroscopy" Blackwell Publishing, USA (2004).
3 J. Kuo, "Electron Spectroscopy: Methods and Protocol" Humana Press, USA (2007).
4 A. Sharma, S. G. Schulman, "Introduction to Fluorescence Spectroscopy", Wiley Interscience, USA (1999).
5 J. P. Glusker, M. Lewis, M. Rossi, "Crustal Structure Analysis for Chemists and Biologists", VCH Publishers, New York, USA (1994).

CHM -799 Modern Trends in Symmetry and Group Theory

Symmetry elements and symmetry properties. Group Algebra. Point groups. Classes Symmetry Reducible and irreducible representations. Matrix algebra and its application in group representation. Character Tables. Applications of group theory in spectroscopy and molecular orbital theory.

Books Recommended:

1. Robert L. Carter, Moleculer Symmetry and Group Theory, Wiley and Sons, 2014, USA
2. Alan Vincent, Molecular Symmetry and Group Theory (2^{nd} Edn), Wiley and Sons, USA, 2010.
3. Mohammad A. "Application of Symmetry and Group Theory in Chemistry" University Grants Commission, Islamabad, 1984.
4. Lesk, A. M. "Introduction To Symmetry And Group Theory For Chemists" Kluwer Academic Publishers, 2004.

PHYSICAL CHEMISTRY

CHM-781 Physical Chemistry of High Polymers 3(3-0)

Molecular forces and chemical bonding in polymers, configuration and conformation of polymer chains, theories of polymer solutions; phase separation and fractionation, plasticization, molecular size measurement, spectroscopic analysis, thermal analysis, morphology and order in crystalline polymers, polymer reheology, electrical and magnetic properties of polymers.

Recommended Books:

1. Flory, "Principle of Polymer Chemistry" Cornell University press, New York, USA (1953).
2. Fried J. R. "Polymer Science and Technology"2nd Ed., Prenitce Hall, USA (1995).
3. Young, R.J. "Introduction to Polymers". 2nd Ed., Chapman and Hall Ltd, UK (1981).

CHM-782 Complex Extension of Quantum Chemistry 3(3-0)

Revision of basic quantum (Historic background, Uncertainty principle, Time-dependent/Time-independent Schrödinger equation, Probability, complex number, Particle in one dimensional box, Tunneling, Operators) Particle in three dimensional box, Requirements of an acceptable wave function, The Harmonic oscillator (one-dimensional harmonic oscillator, Vibration of molecules, Numerical solution of one-dimensional Schrödinger equation), Angular momentum, The Hydrogen atom , Theorems of quantum mechanics (Hermitian operator, Parity, Matrices), The Variation Method (Variation theorem, Determinants, Linear variation methods), Perturbation Theory (Non-degenerate perturbation theory, Perturbation treatment of the Helium atom ground state, perturbation theory for a degenerate energy level).

Recommended Books:

1. I. N. Levine. "Quantum Chemistry, fifth edition" Prentice-Hall, Inc. Upper Saddle River, New Jersey, USA (1991).
2. J. P. Lowe, K. A. Peterson. "Quantum Chemistry" 3rd Ed, Elsevier Academic Press, Netherland (2006).
3. P. A. Cox, "Introduction to Quantum Theory and Atomic Structure", Oxford University Press, UK (2002).
4. P. W. Atkins. "Molecular Quantum Mechanics" Oxford Univ. Press, Oxford, England (1983).
5. M. Muller. "Fundamentals of Quantum Chemistry", Kluwer Academic Publishers, Boston, USA (2001).