Imperial College London

Department of Chemistry

Fourth Year Syllabus

2004 - 2005

Contents

Page

Introduction to Fourth Year Chemistry.....**3**

Inorganic IV

Lecture synopses..... **4**

Organic IV

Lecture synopses..... **12**

Physical IV

Lecture synopses..... **29**

Department of Chemistry – Imperial College

INTRODUCTION TO FOURTH YEAR CHEMISTRY

Aims

The final (usually 4th) year of the MSci courses is designed to bring together what has been learned in the preceding years and to give the opportunity for in depth study of specialist chemistry. As much freedom of choice as is possible within timetabling constraints is given to the students. Much of the year involves a significant practical element in the form of an extended research project. The research project can be selected by the student from a large number of topics, covering all branches of Chemistry. Just over half of the marks for the final year are awarded for this research work, reflecting the great importance of research in the wider sphere of Chemistry. The research project runs throughout the year.

Courses offered

Autumn term: 17 lecture courses (133 lectures) are available, comprising 3 Intersectional courses (24 lectures), 4 Inorganic courses (32 lectures), 4 Organic courses (29 lectures) and 6 Physical courses (48 lectures). The students must select 6 courses from these (maximum 48 lectures).
Spring term: 15 lecture courses (119 lectures) are offered, comprising 3 Intersectional courses (21 lectures), 5 Inorganic courses (40 lectures), 6 Organic courses (42 lectures) and 2 Physical courses (16 lectures). The students must select 6 courses from these (maximum 48 lectures).

Oral Exam

In the spring term, the students are required to undertake an oral examination on selected topics from the first three years of study (topics for examination are posted at the beginning of the Spring Term). The aim of the oral examination is to emphasize the importance of core Chemistry and to give the student practice valuable for future interviews. The mark for the oral examination makes up 6.25% of the year total.

Inorganic IV

Supramolecular Chemistry of Nanomaterials

Steinke, Joachim

8 hours

Aims
This course aims to demonstrate the importance of supramolecular (non-covalent interactions) for the assembly of complex nanomaterials.

Structure
Lecture 1 – Introduction to supramolecular chemistry and nanomaterials. Definition and examples of the main intermolecular forces used in supramolecular chemistry. Scope of the course and the topic.
Lecture 2 – Self-assembly processes in organic systems. Catenanes, rotaxanes, pseudorotaxanes. Synthetic strategies for their preparation. Main supramolecular forces involved in such assemblies. Examples of each type.
Lecture 3 – Self-assembly processes in metal-containing compounds. Self-assembly of metal nanoparticles (via H-bonding and electrostatic forces). Using the coordination bond to prepare large supramolecular assemblies. Cages, macrocycles and catenanes. Polymeric materials and grids.
Lecture 4 – Nano-capsules and containers. Discussion of main synthetic strategies for their preparation. Examples of each type. Potential uses of such assemblies as nano-reactors and for transport (e.g. drug-delivery).
Lectures 5 and 6 – Molecular switches and machines. Use of supramolecular forces to assemble components that respond (on-off) to external stimuli. Molecular shuttles, abacus and muscles. Assembling such components into surfaces for molecular electronics.
Lectures 7 and 8 – Supramolecular chemistry of polymeric materials and in the solid state. Self-assembled monolayers. Molecularly imprinted polymers.

Objectives
By the end of the course the student should have a clear understanding of the importance of intermolecular forces to define the “chemistry beyond the molecule”.
The student should be able to use the basic understanding of such forces to rationalise the formation of complex nanomaterials.
Understand the importance of the bottom-up approach to prepare complex (nanoscale) systems.
The student will be able to recognize the main types of supramolecular assemblies and suggest synthetic strategies for their preparation. Furthermore, the student should be able to identify the main supramolecular forces involved in such systems.

Looking forward to
This material from this course forms the basis for some of the lectures in Designer Ligands (4th year).

Green Chemistry

Williams, Charlotte

8 hours

Aims
The course will focus on the design, development and evaluation processes of green chemistry and is particularly aimed at synthetic chemists or those interested in pursuing environmental chemistry. The principles will be illustrated by specific examples from the recent literature and industry and comparisons will be drawn with traditional methodologies.

Structure
Lecture 1 – Discussion of the current state of chemistry and the environment and the definition of green chemistry. Assessment of the impact of chemistry in the environment and definition of risk and hazard. An introduction to the tools of green chemistry and its fundamental principles.
Lecture 2 – Use of Renewable Raw Materials. Evaluating feedstock and starting materials – their origins, toxicity, sustainability and the downstream implications of the choice of feedstock. Some examples of the use of green starting materials, caprolactam via ammonoximation, commodity chemicals from glucose and biomass conversion
Lecture 3 – Atom Efficient Processes. Evaluating chemical reactions according to their yield and atom efficiency. Examples of efficient stoichiometric and catalytic processes; atom economy and homogeneous catalysis, halide free synthesis and alternatives to the Strecker synthesis
Lecture 4 – Greener Solvents. The use of volatile organic compounds and the need for innocuous replacements. The use of supercritical fluids, solventless, solid supported reagents and aqueous systems as alternative solvents.
Lectures 5 and 6 - Catalysis. Energy requirements and usage, optimization of the reaction by minimizing the energy requirements. Examples of efficient catalytic reactions including the use of heterogeneous catalysis, zeolites and oxidations using molecular oxygen or hydrogen peroxide
Lectures 7 and 8 - Greener reagents and products. Methods of designing safer chemicals such as structure-activity relationships, avoidance of toxic functional groups, minimising bioavailability and use of auxiliary materials. Examples of greener reagents including replacement of phosgene, methylations using dimethylcarbonate, solid state polymerisations, alternative nitrile synthesis. Evaluation of persistence in the environment and examples of biodegradable commercial products; polylactides, polyaspartates and Sea-Nine™ antifoulant

Objectives
By the end of the course students will be able to:
- Evaluate chemical feedstocks, reagents, reaction conditions and target molecules according to the principles of green chemistry
- Propose alternative feedstocks, reagents and target molecules and design syntheses so as to reduce toxicity and environmental impact.
- Discuss the applications for renewable resource raw materials
- Design syntheses of synthetically useful chemicals from polysaccharides, glucose or biomass.
- Calculate the atom economy of a chemical reaction and compare it with the chemical yield
- Assess the replacement of volatile organic solvents with green alternative solvents
- Describe applications for supercritical fluids, solventless processes, solid supported reagents and aqueous solvent systems
- Discuss the role of homogeneous and heterogeneous catalysis in reducing energy consumption.
- Propose suitable catalysts for oxidations using oxygen or hydrogen peroxide and zeolites for acid-catalysis.
- Explain how to design safer chemicals and processes
- Propose safer alternatives to phosgene and applications of dimethylcarbonate
- Recognize how to reduce environmental persistence

Nanotubes

Shaffer, Milo

8 hours

Aims
This course will discuss the structure, synthesis, properties and applications of a range of high aspect ratio nanoparticles. The focus will initially be on carbon nanotubes but will move on to discuss other types of tubular materials, based both on carbon (such as nano-peapods) and other layer materials (e.g. BN, WS2), as well as solid nanorods of metals and, in particular, compound semiconductors. The aim will be to give students a view of the current state of the art and the prospects for future developments. After the course, the students will be aware of the techniques that have been employed to investigate these materials, as well as the difficulties of handling and characterisation.

Structure
Lecture 1: Introduction: Outline, history, examples. Carbon nanotubes: Structure & vectorial definitions. Major synthesis techniques: Key features, variety of products
Lecture 2: Mechanisms: High & low temperature, catalyst selection. Characterisation as applied to nanotubes: TEM, SEM, SPM, Raman, TGA, X-ray. Techniques: Purification, separations, making electrodes, alignment
Lecture 3: Chemistry: Internal, end-cap & sidewall. Non-covalent interactions. Templating reactions
Lecture 4: Properties: Mechanical, electronic, magnetic, thermal, surface-based
Lectures 5 & 6: Applications: composites, nanoelectronics, electrochemical, field emission, catalyst support, sensors, etc
Lecture 7: Analogous structures: doped carbon nanotubes, BN, chalcogenides, oxides. Natural mineral structures. Biological structures
Lecture 8: Nanorods & nanowires. Semiconductor nanowires and the VLS story. Device applications: diodes, memories, sensors

Objectives
By the end of this lecture course, the student should be able to:
- Understand, identify and draw the structures of nanotubes and how they relate to fundamental bulk crystals
- Relate the physical properties of nanotubes to the underlying bonding and symmetry
- Compare and select suitable types of nanotubes for a given application or experiment, taking into account the synthesis route employed
- Propose suitable techniques for purifying, dispersions and assembling a particular nanotube or nanorod device, including characterisation of the result
- Critically assess the prospects for future applications based on nanotubes and nanorods

Modern Applications of Inorganic Chemistry in Industry

Organiser - Davies, Rob

8 hours

Aims
This lecture course is taught by external lecturers from a variety of chemical industries and so its content varies slightly from year to year depending upon the speakers. The aim is to give the students an in depth insight into several specific research areas of topical relevance in industrial inorganic chemistry.

Structure
Structure of the course varies depending upon the availability of industrial lecturers, however last years course (2003-4) covered:

- Performance criteria and cost considerations in catalyst design
- Olefin dimerisation catalysts
- Silicones (chemistry, production and applications)
- Automotive pollution control
- PEM Fuel Cell systems
- The chemistry of light olefin production

Objectives
By the end of the course students should understand and be able to discuss industrial issues for the following topics:

- Performance criteria and cost considerations in catalyst design
- Olefin dimerisation catalysts
- Silicones (chemistry, production and applications)
- Automotive pollution control
- PEM Fuel Cell systems
- The chemistry of light olefin production

Designer Ligands

Long, Nick

8 hours

Aims
To give an understanding of how the properties of ligands can be tuned in order to optimise the performance of metal complexes in their various applications. The origins of these influences will be explored along with an examination of the relevance of these systems to catalytic, biological, chemi-architectural and industrial processes and applications.

Structure
Lectures 1 and 2: Revision of ligand types, their metal complexes and their applications. Why we design new ligands. Focus on phosphines and their importance. Some tunable properties of ligands: basicity, steric bulk, solubility, chirality, denticity etc. The iterative process of design and evaluation.
Lectures 3 to 5: The design and application of functionalised phosphines for homogeneous catalysis: asymmetric hydrogenation. The use of metallocenyl systems for molecular recognition and chiral metallocenes for catalysis (using chiral ferrocenyl-phosphines and -aminoalcohols and chiral group 4 bent metallocene species). Applications of organometallic materials, in particular, metallocene derivatives for nonlinear optics.
Lectures 6 to 8: The application of ligand design to molecular recognition, crystal engineering and self-assembly (via intermolecular interactions, hydrogen-bonding and metal complexation i.e. 'supramolecular chemistry'), featuring systems such as catenanes and helicates.

Objectives
By the end of the course, students should understand how the various properties of ligands may be tuned by design, appreciate the wide-ranging applicability of ligand design and be able to recognise the design elements present in a given designed ligand.

Building upon
This material from this course builds upon Transition Metal Chemistry and Organometallic Chemistry (2nd year), Inorganic Mechanisms and Catalysis (3rd year), Advanced Organometallic Chemistry (3rd year) and Supramolecular Chemistry (4th year)

Ionic Liquids

Welton, Tom

8 hours

Aims
This course is intended to introduce ionic liquids as solvents for synthesis and catalysis applications. However, aspects of their structure and physical properties are included so that a full understanding of their behaviour can be achieved.

Structure
- What is an ionic liquid? Models of molten salt formation and the thermodynamics of melting. Structural influences on the melting point of a salt (2 lectures)
- Physical properties of molten salts and ionic liquids, polarity, interionic bonding, structure (2 lectures)
- Applications of ionic liquids to synthesis. Effects on reaction mechanisms. Acid catalysed reactions (2 lectures)
- Applications of ionic liquids in catalysis. Hydrogenations, oxidations and C-C coupling reactions (2 lectures)

Objectives
By the end of the course, students should:
- Have a thorough understanding of the structure of ionic liquids
- Be able to rationalise the effects of the ionic environment on the properties of solute species, particularly their reactivity.
- Be able to demonstrate a knowledge of the range of reactivities studied in ionic liquids.

Building upon
Non-Aqueous Solvents. The course assumes a knowledge of the material covered in this 3rd year course.

Exploring Inorganic Chemistry

Hunt, Tricia

8 hours

Aims
To feel comfortable reading, and to understand in a broad sense, something of the theoretical component of a combined synthetic/theoretical paper. To have a general idea of the physical properties that can be calculated, and how they can help you in interpreting spectra or analysing mechanisms. To understand how molecular orbitals can be used as an aid for interpreting chemical bonding and reactivity. To be able to evaluate the accuracy of such information. To develop an understanding of potential energy surfaces, how they are explored, and represented, and what relationship they bare to a reaction path.

Structure
The structure of this course has not been finalised and may differ slightly from the outline given below.

- 1-2 Common computational methods used in the study of inorganic systems
- 3-4 Physical Properties
- 5-6 Molecular Orbitals and Bonding
- 7-8 Potential Energy Surfaces and Reactivity

Objectives
- To be able to identify and distinguish (at a gross level) the different types of computational method generally applied to inorganic systems. To be able to describe the advantages and disadvantages associated with each method. To have a feeling for the accuracy of a particular method.
- To be able to outline the physical properties that can be calculated using quantum chemical methods. To be able to describe the accuracy with which these can be predicted, and to have a feeling for the difficulties inherent in calculating different physical properties.
- To be able to interpret and evaluate pictures of molecular orbitals, especially HOMOs and LUMOs. To be able to interpret the results of a population analysis. To be able to use the above mentioned MOs and population analysis to gain insight into chemical bonding and reactivity. To understand the physical relevancy of such information.
- To describe in words what a geometry optimisation, a trajectory and a minimum energy path are. To be able to explain, in words, the key types of critical points that occur on potential energy surfaces; minima, transition state, intermediate, and conical intersection.

Links
This course provides a link between the models of bonding, structure and reactivity invoked in synthetic inorganic courses and the more mathematically detailed and theoretical content of purely physical courses. This paper uses concepts of bonding and structure first introduced in years 1 and 2 and endeavours to link them with the results of calculations carried out using methods that will have been introduced in the computational physical courses of years 3 and 4.

Recommended texts
Further texts will be identified at the beginning of the course.
Why Chemical Reactions Happen, J. Keeler and P. Wothers, Oxford University Press
Introduction to Computational Chemistry, Frank Jensen, John Wiley and Sons

Organic IV

Advanced Polymers

Britovsek, George; Steinke, Joachim and Law, Robert

7 hours

Aims
To introduce students to some of the most significant recent developments in the synthesis of advanced polymers.

Structure
Lecture 1 - GB
Lecture 2 - GB
Lecture 3 - GB
Lecture 4 - Synthetic Strategies for Polyrotaxanes Synthesis Part 1: Definition of rotaxane types. Historic perspective. Threading, slipping, clipping, entering, various forms of stoppering used in the synthesis of rotaxanes and extrapolated to main chain and side chain polyrotaxanes.
Lecture 5-6 - Synthetic Strategies for Polyrotaxanes Synthesis Part 2/Synthetic Strategies for Conjugated Polymer Synthesis Part 1: Polyrotaxanes continued. Introduction to conducting polymers. Synthesis of conjugated (electron) conducting polymers, precursor routes, transition metal catalysis. Syntheses of polyacetylenes, polyphenylenes, polyphenylenevinylenes, polyphenylacetylenes, polythiophenes, and polypyrroles.
Lecture 6-7 - Synthetic Strategies for Conjugated Polymer Synthesis Part 2/Nanowire Synthesis: Conjugated polymers continued. Examples of electro-active (pseudo)polyrotaxanes. Discussion of encapsulation issues for conjugated polymers. Discussion of state of the art progress using the latest developments as basis.

Objectives
By the end of the course the students should be able to

- design suitable starting materials and to select the most appropriate synthetic strategy based on retrosynthetic analysis to synthesise pseudorotaxanes, rotaxanes and their polymeric counterparts.
- Design suitable monomers after retrosynthetic analysis in order to synthesise any given conjugated polymer with particular emphasis on polyacetylenes, polyphenylenes, polyphenylenevinylenes, polyphenylacetylenes, polythiophenes, and polypyrroles.
- Exemplify the synthetic considerations that have to be addressed in order to successfully synthesise encapsulated conjugated polymers (organic nanowires).

Building upon
3.I1 Inorganic Mechanisms and Catalysis 3.I3 Advanced Organometallic Chemistry, 3.I5 Palladium Catalysis in Organic Synthesis - 8 hours, 3.I9 Chemistry of Macrocycles, 3. I10 Non-Aqueous Solvents, 3.O? Polymers: The essential guide, 3.O4 Reactive Intermediates 1 – Radicals, Advanced Stereochemistry 3, Properties of Polymers, 3.An3 Sensing and detection, 3.P9 Molecular Electronics

Looking forward to
Independent Research and Advanced PG courses.

Chemistry of Medical Imaging

Terry Spinks, Gavin Brown, Maria Constantinou, Matthias Glaser

7 hours

Aims

- To provide students with an overview of the principles behind medical imaging with an emphasis on radiochemistry but also covering the basic principles of particle accelerators, radioisotope production and medical imaging devices.
- To provide an understanding of the radiochemistry used or incorporating radioisotopes into compounds of clinical interest and to gain some insight into the applications of these radiopharmaceuticals.

Synopsis

Two introductory lectures will cover the spectrum of medical imaging. The underlying nuclear physics, principles of particle accelerators, radioisotope production and medical imaging devices. Two lectures will illustrate the chemistry used for synthesising radiopharmaceuticals labelled with carbon-11. Two more lectures will illustrate the use of fluorine-18 for synthesising radiopharmaceuticals. The final lecture will cover the syntheses of radiopharmaceuticals labelled with radiohalogens and radiocations. A visit to the PET centre at Hammersmith Hospital will be arranged.

Structure

Lecture 1. Introduction

Spectrum of medical imaging – PET, SPET, MRI, CT Bohr model of atom, definitions of isotope, nuclide. Origins of radiation. Equations for nuclear decay, half-life, graphical determination of half-life. Mechanisms for radioactive decay. Interactions of radiation with matter. Imaging with single photon emitters (SPET). Imaging with positron emitters (PET) Basic design of PET scanners

Lecture 2. Background

Nuclear reactions . Energetics of nuclear reaction. Reaction cross-sections. Nuclear reactors. Radionuclide Generators. Basic mechanisms of cyclotrons. Production of radionuclides.

Lecture 3: Carbon –11 (I).

Stages in the preparation of labelled compounds used in PET studies. The main nuclear reactions and some typical production parameters for carbon-11. Practical considerations in radiochemistry with carbon-11. The direct utility of [11C]carbon dioxide as a labelling agent. The use of [11C]carbon dioxide to prepare mono- and bifunctional labelling agents.

Lecture 4: Carbon –11 (II).

Comparison of the utility of [11C]methane and [11C]carbon dioxide as primary cyclotron-produced precursors. Use of [11C]methane to produce mono- and bifunctional labelling agents. Examples of ring closure reactions using bifunctional labelling agents. Labelling strategies and practical considerations in choosing the position of labelling in target compounds.

Lecture 5: Fluorine-18 (I).

Most commonly used isotopes. Definitions. Properties of fluorine-18. Nuclear production of [18F]fluoride, important radiopharmaceuticals labelled with fluorine-18. Advantages/disadvantages of [18F]fluoride. Factors affecting [18F]fluoride for nucleophilic substitution. Introduction of fluorine-18 into aromatic rings, non-nucleophilic labelling derived from [18F]fluoride. The radiosynthesis of some important radiopharmaceuticals.

Lecture 6. Fluorine-18 (II).

Production of [18F]fluorine. Non-nucleophilic (“electrophilic”)radiofluorination chemistry. Disadvantages of [18F]fluorine. Fluorination reactions with [18F]fluorine electrophilic addition and electrophilic aromatic substitution and some examples. The radiosynthesis of 6-[18F]L-DOPA, and an examples of PET imaging with this and other fluorine-18 labelled compounds.

Lecture 7: Other Radionuclides for Biomedical Imaging.

Properties and production of iodine and bromine radioisotopes, their medical applications in imaging techniques, Overview on direct and indirect labelling protocols for radiohalogens, Role and

chemistry of technetium-99m in nuclear medicine, some other radionuclides for medical imaging, examples of PET and SPECT images from oncology and neurology.

Objectives

By the end of the course the students should be able to appreciate the principles underlying medical imaging and in particular understand the radiochemistry used for producing radiopharmaceuticals as well as having some insight into clinical applications of the latter.

Chemistry and Engineering of Polymers

Law, Robert; Steinke, Joachim; Higgins, Julia; Alpay, Esat

10 hours

Aims

- To highlight the three cornerstones of polymer science: Polymer (Synthesis + Characterisation), Processing and Properties.
- To illustrate the complex interaction needed between Chemistry and Chemical Engineering to produce a polymer product.

Synopsis

The course is designed to discuss the challenges of turning a polymer into an industrial product by considering the entire process covering monomer synthesis, polymerisation chemistry, polymer structure (solution and solid state), morphology and processability. The course consists of three interwoven parts; 8 seminars/2 tutorials and a short laboratory course (2 extended mornings synthesis, 2 extended mornings characterisation/properties/processing). The seminars and tutorials will introduce fundamental aspects of polymer chemistry and polymer chemical engineering with speakers drawn from both the academic and the industrial community. The short laboratory course will provide an opportunity to get hands on experience of aspects of polymer synthesis, characterisation techniques and a basic "feel" for polymer properties.

Structure

Lectures, Synthesis Lab, Characterisation Lab, Processing Lab, Virtual Process Design, Industrial Speaker

Lecture 1. Introduction – Polymer properties. MW, MWD, chain entanglement, random coil, reptation, crystallinity, viscoelasticity.
Lecture 2. Polymer Synthesis: Chain growth, step growth, tacticity, Carothers' equation, kinetics and thermodynamics of polymerisation.
Lecture 3: Polymer Characterisation: GPC, MS, DSC, TGA, NMR, IR.
Lecture 4: Scale-up Issues and Reactors 1: Batch vs continuous. Plug flow, residence time, radial distribution, affect on polymer properties and structure.
Lecture 5: Scale-up Issues and Reactors 2:
Lecture 6: PPP - Structure/Property Relationships in Polymers: Tg, Tm, chemical and thermal stability, viscoelsticity and how these are related to polymer structure (MW, MWD, tacticity etc.)
Workshop 1: Workshop/Tutorial: To provide support and more detailed explanations for the theoretical part of the lab experiments and the associated write-up.
Lecture 7: Polymer Processing: How polymer properties impact on their successful processing into consumer materials. How can a change of synthesis and thus molecular parameters be used to not only improve processing but also to produce new and different products.
Workshop 2-4: Workshop / Case Study: Based on an example of an existing plant, students are divided into groups that are asked to analyse the design of the plant and through this analysis identify shortcomings and limitations of the design itself. They are also asked to make suggestions for improvements and to justify their choices on technological, economical and environmental grounds.
Lecture 8: Industrial Seminar: An industrialist with direct experience in the issues related to the synthesis and scale-up of a polymer product presents the inside view, emphasising points that have been highlighted throughout the lectures given by the academics. A post-lecture mixer allows students to ask further questions

Chemistry of Gene Therapy

Miller, Andrew

6 hours

Aims
This course aims to show how the solution to successful genetic therapies is very much a chemical biology problem at heart. In other words, chemistry is central to the realization of this new and potent therapeutic modality, in particular by making an interdisciplinary combination of careful synthetic and biophysical chemistry.

Structure
- Overview of the importance of chemistry to gene therapy (1 lecture)
- Initial development of synthetic non-viral vector systems for gene therapy (1 lecture)
- Creation of synthetic non-viral vector platform systems; including an introduction to lipid and peptide chemistry (2 lectures)
- Discussion about the physical techniques required to study vector structure and integrity; techniques to follow delivery of nucleic acids to cells in vitro and in vivo (1 lecture)
- Comparison of synthetic non-viral with viral vector systems (1 lecture)

Objectives
By the end of the course the students should be able to:
- Appreciate the importance of chemistry to genetic therapies research.
- Understand the barriers to successful genetic therapies and appreciate how these barriers might be overcome by judicious use of synthetic and biophysical chemistry.
- Appreciate the basic principles behind the physical techniques used to study vector system structure and efficacies.

Advanced NMR Spectroscopy

Law, Robert

7 hours

Aims

- To reinforce and consolidate existing materials learnt in the previous years.
- To provide the students with the understanding of aspects of advanced NMR theory and practice, especially in relation to the solid state.
- To understand the particular problems of NMR in the solid state and which strategies are employed to overcome them.
- To apply simple ideas to understand the nature of the magnetism in the solid state.

Structure

- Summary of current NMR knowledge
- Issues in the solid state
- Mitigation of solid state interactions
- Theory of pulse sequences
- Application to a variety of systems
- Interpretation of solid state NMR spectra

Objectives

By the end of the course the students should be able to

- Understand the aspects of theory of NMR spectroscopy in the solid state
- To understand how to overcome particular problems associated with the solid state
- To interpret basic solid state NMR spectra

Molecular Recognition in Chemical Biology

Miller, Andy

8 hours

Aims
This course aims to build upon the previous course O4 Introduction to Chemical Biology (Year 3) in order to transform an appreciation of biological macromolecular structure into an appreciation of biological function at the molecular level. This course sits alongside and complements the course O7 Chemistry of enzymes, together with other Year 4 courses with a chemical biology/biological theme.

Structure
- Overview of the importance of molecular recognition processes to biology (1 lecture)
- Overview of the forces involved in molecular recognition processes in biology (1 lecture)
- Molecular recognition models, Ka and Kd, thermodynamic relationships (1 lecture)
- Techniques to study and quantify biological molecular recognition processes including resonant mirror biosensor and CD/fluorescence/NMR spectroscopy (2 lectures)
- Case studies in biological molecular recognition processes including molecular chaperone-substrate molecular recognition processes and sense/complementary peptide interactions (3 lectures)

Objectives
By the end of the course the students should be able to:
- Appreciate the importance of molecular recognition processes in biology.
- Understand models of molecular recognition and how to obtain a quantitative measure of these recognition processes.

Biosynthesis and Biomimetic Total Synthesis

Spivey, Alan

7 hours

Aims
To explain the formation of the major classes of secondary metabolites and some primary metabolites; the chemical mechanisms of many of these transformations, with the emphasis on cofactor reactivities; and the way in which these transformations can be used for enantioselective chemical synthesis.

Scope
The lectures will cover:—

- Introduction to course and enzyme cofactor chemistry.
- Biosynthesis of fatty acids and polyketides.
- Biosynthesis of terpenes and steroids.
- Biosynthesis of alkaloids.
- Biomimetic polyketide synthesis
- Biomimetic terpene synthesis
- Biomimetic alkaloid synthesis

Objectives
On completion of this course you will be able to:

- recognise the structural affinities of major classes of natural products;
- appreciate the biological and chemical origins of these compounds;
- offer rational mechanistic explanations of many of the transformations;
- understand the challenges involved in biomimetic synthesis

Combinatorial and Solid Phase Synthesis

Braddock, Chris

6 hours

Aims
To introduce the concept of combinatorial chemistry and the increasingly important role of solid phase synthesis, reagents and scavengers in contemporary organic synthesis.

Structure
1. Introduction to Combinatorial Synthesis: Introduction; Merrifield synthesis of peptides; mix and split for combinatorial synthesis of peptides; deconvolution; orthogonal libraries;
2. Combinatorial Synthesis on the solid phase: Advantages; Resins: type and properties; Linkers; Selected Solid Phase Syntheses;
3. Combinatorial Synthesis in solution: Parallel synthesis; Indexed libraries; Dendrimers; Fluorous phase; impurity annihilation;
4. Encoded methods for Combinatorial Synthesis: Chemical tags; radio frequency tags; multiple release via orthogonal linkers;
5. Analytical techniques for Combinatorial Synthesis: On and Off Bead analysis;
6. Solid supported reagents: Case studies - syntheses of carpanone and epibatidine.

Objectives
At the end of this course students should be able to describe:
- The role of combinatorial chemistry in the drug discovery process
- The advantages of solid phase combinatorial synthesis
- Examples of resin beads used in solid phase synthesis
- The types of linkers employed in conjunction with solid supports
- The type of chemistry that can be employed on solid phase
- The concept of encoded combinatorial synthesis
- Solution phase alternatives to solid phase synthesis
- Analytical techniques for on-bead and off-bead characterisation
- Identify solid-supported reagents

Advanced Heterocyclic Chemistry

Braddock, Chris

8 hours

Aims
To provide a survey of some of the modern methods of heterocycle formation in organic chemistry. The course does not seek to give a comprehensive guide to all the possible methods of heterocycle formation and steers clear of the "classical" methods of heterocyclic formation.

Structure
1. Case Studies. a) Sildenafil: the chemistry of pyrazoles and pyrimidones; b) Thiangazole and Muscoride A; the chemistry of thiazoles and oxaloles; Burgess reagent; Dess-Martin Periodinane; electrophilic phosphorous reagents; DCC; hypervalent iodine reagents.
2. Modern synthetic cyclization methods. a) "Neutral" cyclisations: ring-closing metathesis; McMurry reaction; Palladium catalysed methods as exemplified by the Heck reaction, rhodium carbenoids, aza Wittig reaction. b) Cationic cyclisations: Iminium ions; N-Acyl iminium ions; oxonium ions; spiroketals; heteroatoms as nucleophile. c) Anionic cyclisations: unsaturated alkyl lithiums; furan and pyrrolidine formation; Sn-Li exchange; T.S.; diastereoselectivity
3. Cycloaddition reactions. Multi-component systems; Intramolecular Diels-Alder reactions.

Objectives
At the end of this course students should be able to:
- Identify methods for heterocycle formation within the scope of this course,
- Predict the heterocycle product from a given substrate and reagent,
- Provide reagents for the transformation of acyclic systems into heterocycles,
- Select reagents for the preparation of heterocycles from other substrates,
- Explain the mechanistic rationale underpinning the above.

Pharmaceuticals

GSK

6 hours

Aims
To provide introduction to medicinal chemistry and related subjects in the pharmaceutical industry, presented by experts from GlaxoWellcome.

Structure
Lecture 1: describes the overall processes of the pharmaceutical industry from a chemistry perspective, beginning at the identification of new disease targets, through to the final marketing of a drug, and focuses on the issues and hurdles that need to be overcome at each stage. Changes underway in the industry to minimise the risks of failure at each stage are also described.
Lectures 2-4: Two case study lectures focus on recently developed drugs, illustrating their discovery and the medicinal chemistry challenges and hurdles that needed to be overcome. To support these lectures, a further lecture covers the importance of understanding the pharmacokinetics and metabolism of drug substances, and looks at the effects of physical characteristics and chemical structure on these parameters.
Lecture 5: provides an introduction to the chemical issues around process development of drug substances and scale up from research quantities through to manufacture of drug substances.
Lecture 6 is on newer technologies now impacting on the industry, primarily looking at high throughput screening methods, the generation of compound libraries for screening and the introduction of combinatorial and parallel processing in chemistry at all stages of the drug discovery process.

Objectives
At the end of the course, students should appreciate the factors involved in the discovery and development of modern pharmaceuticals, and be able to select appropriate drug candidates and processes from unseen "case studies".

Chemistry of Enzymes

Robin Leatherbarrow

8 hours

Aims
This course aims to provide an understanding of the way that enzymes catalyse chemical reactions

Structure
- Comparison of enzyme-catalysed and solution reactions
- Kinetics of enzyme-catalysed reactions (Michaelis-Menten kinetics / mechanism; Briggs-Haldane mechanism)
- Allosteric kinetics
- Enzyme inhibition (competitive, non-competitive)
- Reversible / irreversible enzyme inhibitors
- Tight-binding inhibitors and the meaning of IC50
- Effects of pH, temperature on enzyme catalysed reactions; unfolding of proteins/enzymes
- Concept of transition-state stabilisation as applied to enzyme systems and use of transition-state analogues
- Detailed description of several example enzyme mechanisms at molecular detail
- Catalytic antibodies

Objectives
By completion of the course, the students will know the basic equations describing the kinetics of the common enzyme mechanisms and will know how these are affected by the presence of inhibitors. They will appreciate the different classes of inhibitors that are present and know basic factors that influence what makes a “good” inhibitor. Several example mechanisms will have been covered that provide a basis for understanding that enzyme function depends critically on the specific orientation of groups within the active site of the enzyme.

Advanced Synthesis

Barrett, Tony

7 hours

This course will be assessed by project paper rather than by conventional examination.

Aims

To outline and discuss selected total syntheses (six case studies) to illustrate strategic planning, highlighting the use of reagents for asymmetric synthesis and organometallic transformations.

Structure

1. Gilvocarcin (Suzuki): Stereoselective C-glycoside synthesis; benzyne-furan cycloadditions; intramolecular palladium catalysed coupling chemistry.
2. Radicicol Dimethyl Ether (Danishefsky): Sharpless epoxidation; acyl anion equivalents; ring closing alkene metathesis
3. (-)-Histrionicotoxin (Stork) Brown allylboration; epoxide spiroannulation and related reactions; (Z)-iodomethylenylation; Weinreb-Woodward-Vorbruggen amide synthesis; palladium catalysed coupling reactions
4. Strychnine: comparison of Woodward's and Rawal's synthesis Pyrroline-diene Diels Alder reactions; allylation; palladium catalysed cyclisations; isostrychnine synthesis and conversion into strychnine
5. The Endiandric Acid Cascade: Endiandric acids A, B, C and D (Nicolaou): Acetylene coupling; semi-hydrogenation; cascade electrocyclisations and cycloadditions; biomimetic synthesis.
6. (-)-Roxaticin (Rychnovsky): Total synthesis of (-) roxaticin Asymmetric hydrogenation; Brown allylboration; 1,3-dioxanes in stereocontrolled 1,3-diol assembly; polyene construction; macrocyclisation.

Objectives

At the end of this course the student should

- Have an appreciation of the need for strategic planning in the synthesis of complex targets;
- Be aware of some powerful modern synthetic methodologies for the construction of such;
- Be able to plan and devise a possible synthetic strategy to a given target molecule suggesting suitable reagents, highlighting any chemo-, regio-, diastereo- or enantioselection necessary to achieve this end (with the aid of library resources).

Advanced Organic Problems

Craig, Donald

8 hours

Aims
To give the students experience of thinking about and solving demanding problems of stereochemistry, synthesis, mechanism and structural elucidation of organic molecules through spectroscopy.

Structure
Problems classes 1-8: problems are of various types:

- "route-map" problems analysing complex target synthesis sequences
- design of organic syntheses from readily available starting materials
- analysis of published total syntheses in terms of strategy and tactics
- elucidation of unknown products and by-products from real-life reactions from spectra

Objectives
By the end of the course the students should be able to:

- devise strategies for complex molecule synthesis
- think critically about synthetic strategy
- have increased awareness of natural products total synthesis
- apply advanced synthesis thinking in approaches to problems

The Discovery of Agrochemicals

Syngenta

6 hours

Aims
To provide an appreciation of the importance of modern agrochemicals and the factors involved in their discovery. Presented by experts from Syngenta.

Scope
- Introduction: fungicides and bactericides; herbicides; insecticides; plant growth regulators; targeting.
- Lead generation: random screening: DDT; pymetrozine; glyphosate.
- Analogue chemistry: aryloxyphenoxypropionate herbicides. Natural products: pyrethroids; strobilurins.
- Biorational design: juvenoids; pyruvate dehydrogenase; acetylcholinesterase.
- Lead clarification: bioisosteres; sulfonylurea herbicides.
- Lead optimisation - design strategies: structure-activity models; CoMFA; simplex optimisation; agrikinetic properties; propesticides; carbosulfan.
- Compound development - field trials; formulations; toxicology; paclobutrazole; environmental safety; patents. Process research route selection; flufenprox; process development, Manufacture.

Objectives
At the end of the course, students should appreciate the factors involved in the discovery and development of modern agrochemicals, and be able to select appropriate candidates and processes from unseen "case studies".

Catalytic Asymmetric Synthesis

Armstrong, Alan

7 hours

Aims
To explain the principles of catalytic asymmetric synthesis and provide an account of the scope and limitations of current methodology.

Scope
- Introduction and general principles of asymmetric catalysis. Oxidation of functionalised olefins: asymmetric epoxidation of allylic alcohols and enones
- Oxidation of unfunctionalised olefins: epoxidation, dihydroxylation and aminohydroxylation.
- Reduction of olefins: asymmetric hydrogenation.
- Reduction of ketones and imines
- Asymmetric C-C bond formation: nucleophilic attack on carbonyls, imines and enones
- Asymmetric transition metal catalysis in C-C bond forming reactions (cross-couplings, Heck reactions, allylic substitution, carbenoid reactions)
- Chiral Lewis acid catalysis (aldol reactions, cycloadditions, Mannich reactions, allylations); organocatalysis

Objectives
At the end of the course, students should be able to:
- Recognise the types of functional groups which can be prepared by catalytic asymmetric methods discussed in the course;
- Use this knowledge in planning the synthesis of enantiomerically enriched compounds from given prochiral starting materials;
- Outline the scope and limitations of any methods they propose, with respect to parameters such as turnover, substrate and functional group tolerance, availability of catalysts and/or ligands etc

Physical IV

Miniaturised Analytical Chemistry

de Mello, Andrew

8 hours

Aims
Over the last decade that the concepts of miniaturization have been seriously applied to chemical and biological problems. This course reviews the application of these techniques with several illustrative examples, in specific the lab-on-a-chip technology.

Summary
The course begins with a discussion of microscale analytical instruments employing micromachined features (such as channels, electrodes, reactors, and filters). This is followed by a discussion of how they are able to manipulate fluid samples with high precision and efficiency. Microfluidic chip devices have been used in a wide variety of applications including nucleic acid separations, protein analysis, small-molecule organic synthesis, DNA amplification, immunoassays, DNA sequencing, and cell manipulations. In a fundamental sense, these chip-based analytical systems have been shown to have many advantages over their conventional (larger) analogues. These include improved efficiency with regard to sample size, response times, cost, analytical performance, control, integration, throughput, and automation.

The lecture course will provide an overview of the underlying theories and development of lab-on-a-chip systems: the primary aim being to show how the ideas of miniaturisation have begun to fundamentally change the way chemists and biologists work. The course will focus on the theories behind miniaturisation, the methods used to fabricated chips and their application in a wide range of fields (e.g. DNA sequencing, separation science, drug discovery and medical diagnostics).

Objectives
- Students should understand why chemical reactions and molecular separations are highly efficient when performed on the microscale. This involves the understanding of basic electrophoretic theory and molecular diffusion.
- Students will be expected to know how microstructures for chemical analysis are made using conventional micromachining methods (photolithography, wet-etching and bonding) and soft lithographic methods.
- Students will be expected to understand the theory behind and operation of at least two kinds of microdevice for the analysis of DNA and for chemical/biological reactions.

Building upon
Sensing and Detection

Dynamics of complex systems: applications to biology and nanomaterials

Yaliraki, Sophia

8 hours

Aims
This course aims to study the microscopic theories that provide a framework for the understanding of molecular motion and the origin of organization of macroscopic structure from its constituents, central in biology and self-assembling nanomaterials.

Summary
The motivation for this course stems from advancements of micromanipulation techniques to the study of complex systems such as biological and materials at the nanoscale. These experiments have often hinted that collective phenomena are often too complex to be characterized by traditional theories in chemistry typically based on single order parameters or on single reaction coordinates. Furthermore, ubiquitous pair potentials of mean force between small units are insufficient for characterizing the onset of the emerging properties. These new forms of cooperative kinetics offer both a new tool and a scientific challenge. Microscopic theories that provide a framework for the understanding of molecular motions that govern these phenomena are presently lacking; however, they are actively being pursued. Some of the most recent developments will be presented in this course.

- Ensemble and time averages. Time correlation functions. Relevant Probability theory.
- Landscapes of multidimensional systems, stochastic optimization.
- Crossing barriers, rare events & transition path sampling
- Applications to single molecule experiments
- Rare events in quantum systems

Objectives
During this course the student will be introduced to current research questions and will become familiar with different theoretical frameworks. They will become familiar with concepts and methods for setting up the study of complex systems.
By the end of the course they will have acquired skills to evaluate, whence given a problem, whether it is the equilibrium or non-equilibrium behaviour that dominates the system; subsequently to critically choose the most appropriate method for investigation.

Building upon
2nd Year Theoretical Methods, Statistical Mechanics

Protein Function

Klug, David

8 hours

Aims
This course looks a various aspects of protein morphology, how that morphology occurs and the methods used to study it. Specific examples are given of important proteins.

Summary
- Protein location and organisation
- Protein purification
- Protein Stability
- Kinetics of protein folding and the effects of genetic engineering.
- Free energy surfaces and folding.
- Basic enzyme mechanisms and time resolved methods
- Biological catalysis
- Case studies

Objectives
At the end of this course, the students should know the main organelles of cells and have some idea of the contexts in which proteins are found. Simple isolation procedures and the physical principles behind them should be understood along with the strengths and weaknesses of a range of microscopies. The key issues underlying protein stability should be known and the students should be able to express this formally in thermodynamic terms. Experimental methods for measuring the extent and thermodynamics of folding should be known. The transient behaviour of the protein folding process should be understood in terms of free energy surfaces and folding funnels. Experimental procedures to determine the role of particular amino acids should be known along with examples. Students should be able to describe the role of chaperones and the context of folding should be understood. Basic enzyme kinetics should be understood and the Briggs-Haldane equation derived. The students should be familiar with the time course of a simple enzyme reaction and concepts such as Km and turnover number. The students should also be familiar with specific case studies and given examples. Conventional experimental methods for studying the action of enzymes should be known as well as some more particular cases for certain systems including motility assay, pulling experiments and various transient techniques.

Building upon
Biological Chemistry, Interfacial Thermodynamics, Structure and Function in Physical Chemistry.

Mechanistic Photochemistry

Robb, Mike

8 hours

Aims
To understand the mechanistic concepts that control photochemical and photo-physical behaviour in terms of molecular potential energy surfaces

Summary
A photochemical mechanism involves understanding molecular evolution from light absorption to the appearance of ground state products. However photochemistry is complicated by the fact that a reaction path has two segments, one on the electronic excited state and one on the ground state. In addition there is always the competition between radiative pathways (fluorescence) and radiationless decay (internal conversion and inter system crossing). Our objective in these lectures is to understand the mechanistic concepts that appear to control photochemical and photo-physical behaviour in terms of molecular potential energy surfaces. Case studies will be discussed from femtochemistry, organic and inorganic photochemistry, photobiology, photochromic systems, and both synthetic and natural photostabilisers.

Objectives
- to review modern (laser) experiments that show that early theories of photochemical mechanisms were wrong.
- to develop a conceptual basis for mechanistic photochemistry which encompasses the valence bond theory of Excited states, the relationship of the Jablonski Diagram to potential energy surfaces of excited states, the understanding timescales in Photochemistry in terms of electronic and nuclear motion, the understanding of the molecular basis of radiationless decay
- to review new theoretical concepts which provide a general basis for mechanistic photochemistry such as conical intersections and non-adiabatic dynamics
- to study various applications and case studies drawn from laser femtochemistry and coherent control, from “smart” photochemical systems such as photochromic systems, photostabilisers, photochemical and fluorescent switches, from chemiluminescence and from examples in photobiology

Building upon
Photochemistry.

Nanostructured semiconductor materials

Jones, Tim

8 hours

Aims
This course will provide a basic introduction to the growth of semiconductor thin films and the properties of semiconductor thin film structures. The course will introduce the importance of semiconductor thin films in optoelectronic device applications such as light emitting diodes and lasers. The course will cover five main areas:

Summary
This course provides an introduction to the growth and properties of semiconductor thin films. The students will be expected to have a good knowledge of the electronic properties of solids and the physical and chemical properties of solid surfaces. The importance of semiconductor thin films in modern day electronic and optoelectronic devices will be introduced along with the various techniques used for thin film growth. The important role of semiconductor surfaces will be stressed and techniques for monitoring the surface structure and epitaxial growth will be explored, including reflection high energy electron diffraction and scanning tunnelling microscopy. The basic concepts of epitaxial growth will be introduced from a thermodynamic and kinetic perspective and several examples will be used to demonstrate the different growth modes that can occur in lattice matched and lattice mismatched systems. The influence of strain and dislocations will also be introduced. The application of semiconductor thin film structures in optoelectronic devices will be explored, with particular emphasis on the novel electronic and optical properties of quantum well and quantum dot structures.

Objectives
By the end of this course, the students should be able to
- understand the importance of semiconductor thin films in electronic and optoelectronic device applications
- understand the basic principles of semiconductor thin film growth
- explain the structural properties of semiconductor surfaces and the techniques used to monitor them
- explain the different types of growth mode that can occur in lattice matched and lattice mismatched systems
- understand the optical properties of bulk and reduced dimensionality semiconductor heterostructures.

Building upon
Electronic properties of solids, The chemistry of solid surfaces.

Modelling of Nanomaterials

Quirke, Nicholas; Harrison, Nicholas

8 hours

Aims
To introduce students to modelling approaches to nanomaterials, and to demonstrate how these can be addressed by both classical and quantum mechanical approaches

Summary
This course is an introduction to modelling and an overview of its application to nanomaterials. The course starts with an introduction to models in general followed by brief revision of the background statistical mechanics. The first half of the course deals with classical modelling techniques, molecular dynamics and Metropolis Monte Carlo.
The second half deals with electronic structure calculations using density functional theory. The techniques will be illustrated by reference to recent work in the literature.

Objectives
By the end of this course, students should be able to describe the specific issues and challenges associated with the modelling of nanostructured materials, and identify techniques suitable for addressing particular issues.

Building upon
Electronic Properties of Solids. Quantum Chemistry. Theoretical Methods 2.

Optical and electrical properties of nanomaterials

Durrant, James; Yaliraki, Sophia

8 hours

Aims

- Introduce the main processes underlying the optical and electrical properties of nanomaterials
- Compare and contrast the properties of nanostructured materials with bulk materials and with molecular materials
- Illustrate these properties by discussion of specific nanomaterials and nanotechnology applications.

Summary

- Charge Transport: mechanisms, accuracy, control.
- Electronic properties; Size matters: bulk, confined nanoparticles, molecules; Statics, Temperature: Energy levels, Fermi Energy Function.
- Charge Dynamics
- Classical: Ohm's Law, linear response; Tunnelling, Elastic scattering, Landauer; Dissipation, loss of coherence, nonlinear current, temperature.
- Light absorption and emission
- Inorganic nanoparticles: synthesis, quantum confinement, core/shell structures.
- Polymers: Huckel Theory
- Molecular aggregates: J-aggregates.
- Photochemistry
- Supramolecular photochemistry. Photocatalysis. Dye sensitisation of nanostructures.

Objectives

By the end of the course, the students should be able to:

- Identify the primary differences between the optical and electrical properties of nanomaterials compared to both bulk and molecular materials.
- Describe the physical basis of these differences.
- Give examples of how the unique optical and electrical properties of nanomaterials may be exploited.

Building upon

Quantum Chemistry, Electronic Properties of Materials, Molecular Electronics.

Batteries and Fuel Cells

Kucernak, Anthony

8 hours

Aims
To describe the chemical processes occurring within batteries and fuel cells. To elucidate the physical principles that are important in producing batteries and fuel cells which can produce high power and which have (for batteries) high energy densities. To describe the mathematical modelling that can be performed to understand the processes occurring within those fuel cells.

Summary
Primary and Secondary batteries – Lead acid, Nickel Cadmium, Lithium ion and Lithium polymer batteries. Energy density, power density, cycle life. Fuel Cells. How fuel cells work. Different types of fuel cells. Current capabilities/uses. Fuel cell stacks and systems.. Hydrogen as a fuel. Production of hydrogen: Electrolysis, Thermochemical Processes, Steam Reformer Processes, Water Gas Processes, Bosch Process, Biosynthesis and Photochemical Processes, Coal Gasification, Steam Iron Process, Partial Oxidation Processes. Storage, Transport, and Handling of Hydrogen.

Objectives
By the end of the course, the students should have a good understanding the chemistry behind a selection of primary and secondary battery systems. They should understand the aspects of battery chemistry that affect such operating features as capacity, discharge rate, cycle life, and degradation. They should have a good understanding of the different types of fuel cells, and the strengths and weakness of each type. They should be able to perform calculations on the thermodynamics and efficiency of fuel cells operating on different fuels. They will also have a good understanding of the rationale behind the hydrogen economy and the scientific and technical methods used to produce, transport and store hydrogen.

Building upon
Electrochemical dynamics, interfacial thermodynamics.

Complex Solids

Kornyshev, Alexei

8 hours

Aims
With rare exclusion, no physical-chemical processes of practical importance take place in homogeneous media or on flat surfaces. If we benefit from these processes we tend to maximally increase the space where the desired events take place, using rough surfaces or composite media with huge interface area between its components. These as well as many naturally grown structures one might call 'real media'. Such media have typically complex statistical geometry translated into their physical properties and the laws for the processes taking place there. The aims of the course are: To describe the structure of complex solid media such as naturally grown porous rocks, colloid aggregates, man made composites, and rough, volume filling surfaces from catalysts to natural adsorbents or corroded metals. To elucidate the principles of experimental characterization of such systems. To reveal the laws of their growth and the resulting complex structures. To describe the theory of kinetic processes in such structures demonstrating the interplay between the physics and statistical geometry. To consider examples - from colloid chemistry to heterogenous catalysis, electrochemistry and fuel cells.

Summary
Euclidean vs fractal geometry, self similarity. Deterministic fractals, random fractals. Characterization of fractal and non-fractal complex media. Aggregation and growth: from laws to the structures; fractal and nonfractal growth. Theory of percolation. Percolation composites with particle size distribution. Equilibrium properties of complex media and aggregates, absorption and adsorption, electrophysical properties. Processes in complex media; examples: transport phenomena in porous rocks, complex impedance of porous electrodes, performance of electrocatalysts, supercapacitors and composite fuel cell electrodes. Degradation of composite electrodes. Solid polymer electrolyte membranes: proton and water transport.

Objectives
By the end of the course, the students should have a good understanding of the specificity of physics and physical chemistry of the processes in 'real' media, what differs them from the processes in single crystals or any other objects with single structural scale. In particular they should learn a language for complex media characterisation and the principles of experimental study of the features related to complexity. They should be able to give a reasonable guess about the resulting structures based on the laws of their growth. They should be able to understand the laws of percolation and the properties of percolation clusters. They will learn about the transport and reaction phenomena in complex media and should understand what new features may come up as a consequence of our desire to increase the interfacial space, valuable for many applications. They will learn about complex impedance of metal electrolyte systems and should be able to relate experimental data with the stochastic geometry of the system. In the end they will be introduced to the complexity at very short space- and time- scales, using the example of proton conducting ionomers, important for fuel cell applications.

Building upon
2nd Year Theoretical Methods

Electronic Structure Methods

Gould, Ian

8 hours

Aim
Introduction to advanced electronic structure methods, including Hartree-Fock, Density Functional, Moller-Plesset theories. To inform the student of the accuracy, applicability and computational tractability of such methods. Illustration of the uses of the methods and their results to experimental data.

Summary
- Wavefunctions, what are they?
- Development of mathematical formalism of QM
- Basic building block of most theories Hartree-Fock Self Consistent Field equations
- Concept of Basis sets to represent Atomic orbitals and Molecular orbitals.
- Computational implementation and scaling problems with HF-SCF
- Development and application of Configuration Methods, MP2, MP3,CCSD, CASSCF etc
- Introduction of Density Functional Theory
- Brief review of methods to investigate excited states
- Application of methods to calculate molecular properties

Objectives
To be able to:
- define and interpret the underlying principles of QM
- derive the HF SCF equations
- derive expressions for the energies MP2 and CCSD
- critically evaluate referred papers with respect to the level of theory used.
- select an appropriate level of theory, with respect to quality and computational tractability, to study the properties of a wide range of molecules

Building upon
1st Year Quantum Mechanics. 2nd Year Theoretical Methods, Quantum Chemistry

Wetting phenomena: from macroscale to nanoscale interfaces

Dr. F. Bresme

8 lectures

Aims
This course is devoted to wetting from the macro to the nanoscale. The course covers the physical chemistry - chemical physics of static and dynamics of wetting, with particular emphasis on wetting phenomena at the nanoscale. Specific examples and applications to nanomaterials will be discussed.

Summary
- Fundamentals of wetting and capillarity: Surface tension and free energy. Capillarity and gravity (capillary length). Minimal surfaces.
- The three phase line and the line tension: The free energy and the line tension. Beware of the line tension, a small force but not at the nanoscale!. Elasticity of the three phase line. Thermal fluctuations and breakdown of thermodynamics.
- Wetting and long-range forces: van der Waals/electrostatic interactions and solid substrates. Disjoining pressure. Long range forces and the real world: the Healing length, the structure of the three phase line, film stratification. Immersion forces and thin films.
- Dynamics and Wetting: Dynamics of thin films. Dynamics of the three phase line. Dynamics of dewetting.
- Wetting and Transport Phenomena: Chemical gradients. Thermal gradients. Electrocapillarity / Electroosmosis.

Objectives
By the end of the course the students should have a good understanding of the fundamentals of wetting- static and dynamics- and its relevance to industrial processes: flotation, detergency, microfluidics or lubrication. They should understand the differences between wetting at the nanoscale and the macroscale and the importance and uses of immersion forces and long range forces in self organisation of nanostructures (e.g. nanoparticles and proteins). They should be able to use the concepts seen in the course to interpret experimental data in terms of the underlying intermolecular forces acting at interfaces.

Building upon
Interfacial Thermodynamics.