

Postgraduate Courses Timetable

October 2018

Special Postgraduate Courses

Practical computational chemistry (T. van Mourik, H. Fruchtl, M. Buehl, C. A. Morrison, J. Mitchell, D. Rogers)	Semester 1
Resources for Computational Chemistry (H. Fruchtl, short induction course)	Week 1 or 2, Semester 1
Advanced NMR problems (T. Lebl)	May 2017 (TBC)
Powder diffraction for materials chemists (Y. Andreev)	November 2018
An introduction to Fortran (T. Van Mourik)	Semester 2 (TBC)
Electron microscopy (W. Zhou)	Semester 2 (TBC)
Chemistry of sulfur and related elements (R. A. Aitken)	Semester 2 (TBC)

Postgraduate courses based on honours level undergraduate courses

These are (part of) a level 5 undergraduate course, and may therefore not be suitable for St Andrews MChem graduates. Most up-to-date timetable of Honours level courses is available on the School's web site under Current students > Undergraduates > Course resources under - Lecture Timetable

Semester dates for current academic year are at the University website:

<http://www.st-andrews.ac.uk/semesterdates/>

List of courses Semester 1 – Available to sign up for Semester 1

Bioinorganic Chemistry (B E. Bode, CH4514)	weeks 1-5, Semester 1
Second and Third Row Transition Metals, Lanthanides and Actinides (E, Zysman-Colman, CH4514)	weeks 7-11, Semester 1
Homogeneous catalysis (P. Webb, R. Tooze, CH5511)	weeks 1-11, Semester 1
Asymmetric synthesis (A. D. Smith, CH5611)	weeks 1-3 & 5, Semester 1
Advanced spectroscopic techniques (G. Haehner, CH5711)	weeks 1-3, 5,10&11 Sem 1
Laser spectroscopy (C Baddeley, CH5711)	weeks 4, 7-11 Semester 1
Processing of materials (J. T. S. Irvine, C. D Savaniu, CH5716)	weeks 1-11, Semester 1
Nanostructured materials (W. Zhou, M. Buck, CH5717)	weeks 1-11, Semester 1

Semester 2 courses – to be confirmed

Advanced main group chemistry (P. Kilian, A Stasch CH4515)	weeks 1-11 , Semester 2
Electrons and Solids (M. Buck, CH4715)	weeks 1-4 , Semester 2
Functional Materials (F. D. Morrison, CH4715)	weeks 6, 8-11 , Sem 2
Light Interaction with Matter (R. Schaub, CH4717)	weeks 1-5, Semester 2
Solid State NMR (S. E. M Ashbrook, CH4717)	weeks 6-11, Semester 2
Paramagnetic Inorganic Molecules (B. E. Bode, CH5517)	weeks 1-5 , Semester 2
Photophysics of Coordination Compounds (E. Zysman-Colman CH5517)	weeks 6, 8-11 , Sem 2
Blockbuster Solids - Perovskites (P. Lightfoot, CH5518)	weeks 1-5, 11 , Sem 2
Blockbuster Solids – Porous Solids (R. Morris, CH5518)	weeks 5,6,8-11 , Sem 2
Enzyme co-factors (D. O’Hagan, CH5612)	weeks 1-4 , Semester 2
Biosynthesis (T. K. Smith, CH5612)	weeks 4,5,8 , Semester 2
Natural Products (G. Florence, CH5612)	weeks 6, 8-10 , Sem 2
Reactive Intermediates (R. A. Aitken, I. A. Smellie, CH5613)	weeks 1-11 , Semester 2
Chemical Biology (N. J. Westwood, CH5614)	weeks 1-11 , Semester 2
Molecular Recognition (E. R. Kay, CH5616)	weeks 1-11 , Semester 2
Surface Science (C. J. Baddeley, CH5713)	weeks 6, 8-11 , Sem 2
Heterogeneous catalysis (P. Wright, CH5713)	weeks 1-5 , Semester 2
Chemical applications of electronic structure calculations (M. Buehl, J. Mitchell, CH5714)	weeks 1-11 , Semester 2
Energy Conversion and Storage (J. T. S. Irvine, R. T. Baker, A. R. Armstrong CH5715)	weeks 1-11 , Semester 2

Transferable skills training courses

PhD Thesis writing: to be held at the University of Edinburgh at the beginning of Semester 2, date and time to be confirmed (a single day course, transport provided, carries one credit, recommended for 3rd year PG students).

Academic Paper writing: to be held in St Andrews in Semester 2 – normally around June/July, date and time to be confirmed (a single day course, carries one credit).

Course Abstracts

Special Postgraduate Courses

Practical Computational Chemistry (*Wednesdays, 1.00-2.00pm, Physics room 307, course starts 10th October and runs for 9 weeks including Independent Learning week*)

A practical course to introduce graduate chemistry students (and other chemistry researchers) to computational chemistry techniques. Assignments will be carried out on the EaStCHEM Research Computing Facility, but the concepts and skills gained will be generally applicable. The course will be run over the SUPA network using speakers from both Edinburgh and St Andrews Universities.

Registration: Please give name, email address and name of supervisor to Tanja van Mourik (tanja.vanmourik@st-andrews.ac.uk). Postdocs or staff who plan to attend should also register, because they need a SUPA account to access the material.

Syllabus:

Basic theory behind ab initio, DFT, semi-empirical and classical techniques

Cheminformatics

Introduction to HPC facilities and batch queuing systems

Introduction to Linux and vi

Using visualization tools to set up calculations and analyse the results

Using molecular electronic structure codes - Gaussian and NWChem

Computational Spectroscopy

Using classical simulation codes - Amber and DL_POLY

Using periodic electronic structure codes - CASTEP and CPMD

Resources for computational chemistry (H. Fruchtl, short induction course, 3 lectures, week 1 or 2, Semester 1)

Short induction course on computational chemistry for students who consider using computational methods as part of their research.

Lecture 1: Using the EaStCHEM Research Computing Facility. An introduction to Linux, how to connect to the cluster and run calculations.

Lecture 2: Molecular Quantum Chemistry with Gaussian. An overview of methods and how to use them with Gaussian.

Lecture 3: DFT calculations on periodic systems. An introduction to calculations on materials and surfaces using the programs CASTEP and SIESTA.

Advanced NMR problems (T. Lebl, 6 lectures and practical assignment, May 2018 (TBC), 2 credits)

The aim of this course is to present the most important modern NMR methods used for structure elucidation of small and mid-sized molecules. Although emphasis is on practical application of NMR techniques the introductory session should provide some basic information about physical background of NMR spectroscopy which is essential to gain some understanding of those modern multi-pulse NMR techniques. However, uninviting mathematical description should be avoided using pictorial models. Homonuclear correlations (COSY, TOCSY) and heteronuclear correlation (HMQC, HSQC, HMBC), which are more or less routine nowadays, will be trained and some attention will be also paid to multinuclear application of those techniques. Furthermore, less common techniques such as INADEQUATE and NOESY will be shortly introduced as well. The course will also deal with some other phenomena in NMR spectroscopy such as dynamic processes and relaxation. Furthermore, practical aspects of assignments using MNova software are covered.

Powder diffraction for materials chemists (Y. Andreev, 5 lectures, Semester TBC, 2 credits)

This brief course will outline the principles of the use of X-ray diffraction for characterising crystalline materials. The focus will be on understanding the ideas of crystallographic symmetry and the principles and processes underlying the determination of 'small molecule' crystal structures by single crystal X-ray diffraction. Powder diffraction and macromolecular crystallography will not be covered. St Andrews graduates are welcomed to attend, but will not be awarded credits for this course as the material has been covered in their UG degree.

An Introduction to Fortran (T. van Mourik, 10 lectures, 10 tutorials, Semester 2, 3 credits)

This course teaches the Fortran 90/95 programming language, which is one of the most widely-used programming languages in chemistry. The course is useful for students who need programming skills for their PhD research, but also for any other student who would like to use programming in the course of their research. Access to a computer and Fortran compiler will be provided. No prior programming experience is required.

Electron microscopy (W. Zhou, 6-8 lectures, Semester 2, 2 credits)

The course will introduce the basic principles of electron microscopy and discuss several commonly used techniques for microstructural analysis of solid state materials. Lectures are given on: (1) Introduction, interaction of electrons with the solid; (2) scanning electron microscopy; (3) Energy dispersive X-ray spectroscopy; (4) Electron diffraction and (5) High resolution transmission electron microscopic imaging.

Objectives:

1. To understand the basic ray diagram for an electron microscope.
2. To know the difference between powder X-ray diffraction and electron diffraction.
3. To have some ideas about the interaction of electrons with a solid specimen.
4. To know the principle of SEM.
5. To understand how EDX works.
6. To know some applications of HRTEM.

Chemistry of Sulfur and related elements (A. Aitken, 3 lectures (2 hours each), March 2019, 2 credits)

Position of sulfur in periodic table and comparison of compound types with oxygen. Structure and nomenclature of different compound classes containing S. Syntheses and simple reactions involving thiols, sulfides and disulfides. Thiiranes, thiirenes and their S,S-dioxides, Ramberg-Bäcklund reaction, other 3-membered rings containing S. 1,3-Dithianes and 1,3,5-trithianes, thioesters, dithioesters and thiocarbonates, sulfonium ylides. 1,3-diene / SO₂ adducts - sulfolenes and their use in intramolecular Diels-Alder reaction. Asymmetric synthesis methods using sulfoxides and sulfoximines. Use of ³³S NMR. Sulfur in primary metabolism - biosynthesis and degradation of Cys, Met etc. Sulfur in natural products: Coenzyme A, mammal defence compounds and fruit/vegetable flavours and fragrances including especially onion/garlic family. Other S-containing natural compounds including thiophenes, thiazole amino acids, polysulfides. Brief treatment of the use of selenium compounds in organic synthesis.

Postgraduate Courses based on Honours level Undergraduate Courses

Bioinorganic Chemistry (B. E. Bode, 10 Lectures, Theatre C, 2 Credits)

This course provides an understanding of the mechanisms of electron transfer reactions and their importance in the catalytic reactions of metal containing biological systems.

Content and Objectives:

1. To understand why electron transfer reactions are important and to be able to discuss different methods to study them.
2. To know the principles of electron transfer mechanisms:
 - a. Outersphere electron transfer
 - b. Innersphere electron transfer
3. To appreciate the relation between thermodynamics, kinetics and quantum theory (Marcus theory).
4. To know that these mechanisms are operative in biological systems (Respiration, DNA, Photosynthesis)
5. To be able to discuss the tunable versatility of the Fe-heme system in biology from O₂ binding and transport in hemoglobin (myoglobin) to electron transfer (cytochromes).
6. To be able to discuss the mechanism/structure relationship underpinning the Fe-heme dependent O₂ activation in cytochrome P450.
7. To be able to discuss the structure/function relationship in copper containing proteins involved in O₂ transport and activation
 - a. Type -1 'blue' copper redox proteins
 - b. Plastocyanin and azurin, hemocyanin
8. To be able to analyse the bioinorganic chemistry underlying the nitrogen cycle.
 - a. Fe(S), and Mo in N₂ fixation.
 - b. FeMo protein and FeMo cofactor in bacterial nitrogenase
 - c. Laboratory models
9. To be able to apply the principles developed in this part of the course to related but unseen problems.

Second and Third Row Transition Metals, Lanthanides and Actinides (E. Zysman-Colman, 10 Lectures, Theatre C, 2 Credits)

Aims: This module is intended as an advanced coordination chemistry module and builds upon concepts explored in year 2 modules covering transition metals and coordination chemistry and also bonding and spectroscopy in transition metal complexes. This part of the course explores the lower reaches of the Periodic Table by investigating the chemistry of the 2nd and 3rd row d-block and f-block elements. The coverage of the 'heavier' metals seeks to compare and contrast the properties mentioned above e.g. chemical, spectroscopic and magnetic with those of their lighter counterparts e.g. the first transition series. At the end of the course students should be in a position to fully understand the chemistry of the heavier elements and rationalise the trends in chemical properties both down and across the Periodic Table.

Objectives:

- To explain the concepts behind the chemistry of the 4d and 5d transition elements. The radial and angular expansion in the d-orbitals and the role played by relativistic effects.
- To explain the reasons behind the following: The stability of compounds in very high oxidation states and the formation of covalently-bonded compounds having high coordination numbers. The extensive formation of metal-metal bonded compounds. The greater d-orbital splitting and exclusive formation of low spin complexes.

- To explain the photophysical properties typical 4d and 5d metal complexes.
- To explain the concepts behind photoredox catalysis using 4d and 5d metal complexes as photocatalysts.
- To explain the physical properties, coordination chemistry and electronic configuration of the lanthanides, including trends observed across the periodic table, term symbols, micro-states and the nature of absorption and emission.
- To explain the physical properties, coordination chemistry and electronic configuration of the actinides, including their radioactive character, their absorption properties and trends observed across the periodic table.
- To describe the use of heavy d-block and f-block metal complexes in medical applications, e.g., cisplatin and auranofin.

Homogeneous catalysis (P. Webb, R. P. Tooze, CH5511, 20 lectures, weeks 1-10, Purdie Lecture Theatre D, Semester 1, 3 credits)

The products of catalysis are all around us; it is estimated that >35% of global GDP depends on catalysis. Looking into the future sustainable production is also reliant on catalysis, ensuring efficient utilization of energy and raw materials. The nature of homogeneous catalysts makes them amenable to spectroscopic and computational scrutiny. Advanced synthetic methods allow exquisite control of structure. All this offers the opportunity to design improved catalysts and processes.

By focusing on some detailed case studies this course aims to demonstrate the links between catalyst structure, performance, commercial utilization and sustainability.

Objectives:

1. To revise basic mechanistic transition-metal and organometallic chemistry.
2. To know and understand the elementary steps needed for the construction of a catalytic cycle.
3. To recognise, understand and apply methods based on transition-metal organometallics for the construction and transformation of carbon skeletons.
4. To recognise, understand and apply catalytic and stoichiometric methods of carbonylation.
5. To recognise, understand and apply methods for the elaboration of alkenes.

Asymmetric synthesis (A. D. Smith, CH5611, 10 lectures, weeks 1-5, Purdie Lecture Theatre C, Semester 1, 2 credits)

This course is designed to give postgraduates an introduction to the principles of asymmetric synthesis. It will cover all of the basic concepts that provide the ground rules for most stereoselective reactions, including language, nomenclature and reactivity.

Content and Objectives:

1. To understand the importance of chirality and how to determine the absolute configuration of stereogenic centres and of chiral molecules such as allenes that do not contain stereogenic centres. To understand the function of topicity and the need for prochiral descriptors in stereoselective organic synthesis.
2. To probe the range of stoichiometric methods available for effecting stereoselective synthesis including:
 - a. The use of an existing stereocentre to direct the course of a reaction: examples including the stereocontrol in 6 membered rings, acyclic stereocontrol using 1,3 allylic strain and the use of the Felkin-Anh model to predict the preferred face of nucleophilic attack upon a carbonyl group with an adjacent stereocentre.

- b. To understand substrate directed chemical reactions and their application to epoxidation, cyclopropanation and reduction.
- c. The use of chiral auxiliaries in asymmetric synthesis, and to understand the importance of selective enolate formation. To combine these principles and describe their use in enolate alkylation, aldol reactions and cycloadditions.

Advanced spectroscopic techniques (G. Haehner, CH5711, weeks 1-3, 5, 10 & 11, Purdie Lecture Theatre C, Semester 1, 2 credits)

The course introduces to advanced laser based spectroscopies for the elucidation of structure, properties and reactivity of molecules and materials. It will cover basic aspects of spectra, e.g. what can be learned from the shape of a spectral line.

By discussing various examples, a range of applications of laser spectroscopies will be covered including

1. To learn about particles (atoms, ions, electrons) as advanced spectroscopic tools.
2. To appreciate the opportunities presented by high intensity, polarised and monochromatic radiation over a wide range of photon energies for the characterisation of a material.
3. To understand what a synchrotron is and to appreciate its unique characteristics for spectroscopic applications.

Laser Spectroscopy (C. Baddeley, CH5711, weeks 4, 7-11, Purdie Lecture Theatre C, Semester 1, 2 credits)

Objectives:

1. laser induced fluorescence for studying gas phase kinetics and biomolecules
2. nonlinear laser spectroscopy for surface studies
3. femtosecond chemistry, monitoring bond breaking with ultrashort laser pulses

Processing of Materials (J. T. S. Irvine, C. D Savaniu, CH5716, 20 lectures, weeks 1-11, Purdie room 314, Semester 1, 3 credits)

Advanced functional materials are at the heart of many cutting edge technologies, such as advanced microelectronics or new devices for energy conversion and storage. While the fundamental chemistry and physics of these materials are vital in determining their properties and performance, the final form and microstructure can be equally important in influencing these. This form and microstructure is largely controlled through the processing of the materials and variables such as layer thickness, grain size and porosity can have a profound effect on the final functionality of the material. The aim of the module is to develop an understanding of various aspects of materials processing and how these influence the final form of the material or device. We will concentrate on ceramics processing for thick and thin film devices with a focus on the former as these are central to many of the devices for the applications outlined above and not as well covered in general texts compared to other forms of materials processing such as those for metals and polymers.

Objectives: 1. Be aware of the various types of thick and thin film processing such as tape casting, screen printing, physical deposition methods, sol gel, electrophoretic deposition, how these can relate to different device architectures and the importance of process-performance relationships. Discuss the selection of suitable process methods in terms of overall device design, process integration cost and scalability.

2. Review other paste based processes such as calendaring and extrusion which are useful in the production of supports and substrates. Discuss the advantages and disadvantages of these and where they fit into various process scenarios for devices based on advanced functional materials.
3. Understand the mechanism and kinetic limitations of conventional solid state reactions. Understand the chemistry of sol gel processing and to provide examples of the use of alkoxide and carboxylate precursors to prepare ultrafine oxide powders. To understand the chemistry of intercalation/deintercalation processes, and to provide examples of their importance.
4. Understand the influence of starting powders in slurry and paste based ceramic processing. Discuss how differing powder synthesis routes impact powder properties such as particle size and shape, the impact this can have on pastes and slurry properties and how to modify these by calcination or milling.
5. To be able to discuss the formulation of slurries and pastes for thick film process methods such as screen printing or tape casting. Know the functions of the main constituents in a slurry, preparation methods (such as milling and dispersion), and how to manipulate the formulation and preparation to achieve the desired slurry properties. Compare the advantages and disadvantages of organic versus aqueous based systems.
6. Understand the principles of slurry rheology. Discuss different types of flow exhibited by slurries and what variables can influence this. Understand how to quantify flow in non-Newtonian systems and the importance of measurement technique. Discuss drying of the slurry, the shaping and properties of the green body and how these can influence the final fired ceramic.
7. Understand sintering mechanisms and how raw materials and green body processing influence this. Discuss engineering of microstructures to achieve desired functionality.
8. Understand driving forces for sintering, mass transport mechanisms, and atomic mobility. Solid-state sintering: mass transport mechanisms. Discuss and understand stages of sintering and relation with microstructure development.
9. Understand liquid-phase sintering: thermodynamic and phase equilibria, sintering models, and transient-liquid phase sintering.
10. Reactive sintering processes: reactive sintering, reaction bonding, and reactive hot compaction.
11. Pressure-assisted sintering: effect of pressure in sintering, deformation mechanisms, densification maps, and pressure-assisted sintering processes. Secondary phenomena: phase transformations, Review the effects of constraint on sintering and final microstructure. Application of sintering aids both solid state and liquid phase
12. Control of porosity through slurry formulation, thermal processing and templating. Review graded structures and interfaces, discuss application of composite structures and recent developments in attaining these through infiltration and coating.
13. Case studies of two common thick film processes in more detail, in this case screen printing and tape casting. Review applications of these techniques and understand both the advantages and limitations of each. Be able to discuss the specific slurry characteristics required for each process. Identify some common process issues that may be encountered; be able to suggest possible solutions for these.

Nanostructured Materials (W. Zhou, M. Buck, CH5717, 20 lectures, weeks 1-11, Purdie Lecture Theatre C, Semester 1, 3 credits)

This course is an introduction to the concepts and science behind the design and synthesis of a wide range of nanostructures and the application of these structures in functional materials and devices. The relationship between nanoscale structure and composition and macroscale properties and behaviour will be emphasised.

Objectives:

1. To become acquainted with the idea of nanoscience and nanotechnology
2. To classify the nanomaterials and nanostructured materials in terms of their number of dimensions: clusters, nanoparticles and quantum dots (0-D); nanotubes, nanowires and nanorods (1-D); nanosheets and films (2-D); and porous crystals, mesoporous structures and metal-organic frameworks (3-D). To understand structures of carbon particles, including fullerenes, diamondoids, nanotubes and graphene films.
3. To learn about basic methods for the synthesis of nanomaterials and generation of nanostructured materials involving top-down and bottom-up strategies.
4. To understand the principles of characterization and manipulation techniques for nanomaterials, such as SEM, TEM, AFM, STM.
5. To understand basic principles of nanoscience.
6. To learn about applications related to nanotechnology in sensing, electronic or optical devices, healthcare, and catalysis.
7. To raise awareness for the health and safety issues related to nanomaterials.



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Semester 2 courses

Advanced Main Group Chemistry (P. Kilian and A. Stasch, CH4515, 3 credits)

To discuss the syntheses, structures, bonding modes and selected reactivity of a wide range of molecular main group element compounds from the s- and p-block, including low coordinate mono- and dinuclear species, ring and cage molecules, and main group cluster compounds. The bonding in the different compound classes will be presented and general rules for predicting their geometry will be introduced, e.g. for those of boranes and Zintl anions. Further advanced topics in s and p block chemistry will be introduced, for example the stabilization of heavier main group multiple bonds, low coordinate main group element centres, base stabilised low valent main group compounds, non-classical bonds, frustrated Lewis pairs, weakly coordinating anions and novel s-block metal bases.

Objectives:

1. To know basic electron counting rules for main group and transition metal clusters.
2. To recognise structural similarities of ring, cage and cluster compounds.
3. To know and understand properties and reactivities of selected main group compound classes.
4. To understand the differences and similarities of selected concepts used in organic, organometallic and main group inorganic chemistry.
5. To understand advanced bonding concepts in main group compounds, i.e. 3 center 2 electron, 3 center 4 electron and π^* - π^* bonding.
6. To recognise the importance of ligand properties and steric protection in the synthesis of low coordinate main group compounds including multiply bonded systems and to know the implications for their reactivity.
7. To know a wide range of contemporary chemical concepts and research topics based on compound classes spanning different groups of s- and p-block elements.
8. To understand the link between structure and bonding of various main group compound classes and their reactivity, including small molecule activation.

Electrons and Solids (M. Buck, CH4715, 2 credits)

The module covers electronic structures and properties of semiconductors which, thinking of mobile phones, computers, sensors or solar cells, underlie our modern society. Building on concepts of molecular orbital theory a qualitative understanding of band structures is developed. Characteristic differences in the electrical properties of inorganic and organic semiconductors are discussed on the basis of band type or hopping conduction. The characteristics of intrinsic and extrinsic semiconductors are addressed, as well as semiconductor junctions and the (opto)-electronic properties of organic semiconductors.

Functional materials (F. Morrison, CH4715, 2 credits)

Mobile phones, personal computers, air bags, solar cells: our modern society would not exist without the diversity of properties of dielectrics, semiconductors, and metals. The principal aim of the course is to understand the key properties of these materials and how to enhance their functionality. At the end of the course students will be able to: understand mechanisms for modifying the properties of functional materials, including the influence of defect chemistry and doping on intrinsic and extrinsic conductivity; To appreciate the role of synthesis conditions, particularly partial pressure of oxygen, on the properties of functional oxides; To understand basic

materials selection criteria and basic operating principles for commercial devices including: magnetic, ferroelectric, phase change and multiferroic materials for non-volatile memories, piezo- and pyroelectric devices, microwave dielectric resonators for mobile phones, thermistors and varistors, multilayer ceramic capacitors.

Light Interaction with Matter (R. Schaub, CH4717, 2 credits)

The aim of this course is to develop a greater understanding and appreciation of the way that electromagnetic radiation interacts with small molecules. Fundamental theory of rotational and vibrational spectroscopy will be discussed alongside practical aspects of experimental techniques and methods for obtaining structural information from spectra.

Objectives:

1. To revise the principles of the absorption, emission and scattering of photons by molecules and the nature of excited electronic states.
2. To revise the essential features of the quantum theory of the rotation and vibration of diatomic molecules.
3. To give a simple description of the nature of electro-magnetic radiation and an introduction to the quantum theory thereof.
4. To examine the nature and derivation of the Einstein A and B coefficients related to the rates of absorption and emission of radiation by molecules.
5. To consider the nature of selection rules and discuss in detail how they are obtained for vibration-rotation excitations in diatomic molecules.

Solid State NMR (S. Ashbrook, CH4717, 2 credits)

The aim of this course is to develop a greater understanding and appreciation of the way that electromagnetic radiation interacts with atoms, molecules and solids. Fundamental theory of NMR spectroscopy will be discussed alongside practical aspects of experimental techniques and methods for obtaining structural information from spectra.

Objectives:

1. To understand the important interactions that affect solid-state NMR spectra and, in particular, the differences from solution-state NMR.
2. To understand how line narrowing techniques, such as magic-angle spinning (MAS) and decoupling, work and how high-resolution spectra can be obtained.
3. To understand how structural information can be obtained from solid-state NMR spectra, and to be familiar with of a range of problems and applications where solid-state NMR can be useful.

Paramagnetic Inorganic Molecules (B. E. Bode, CH5517 , 2 credits)

To provide an overview of inorganic 'open shell' compounds including synthesis, characterisation and applications of paramagnetic inorganic species. To survey basic and advanced electron paramagnetic resonance experiments useful for characterisation, determination of molecular and electronic structure and the study of structural dynamics of paramagnetic molecules.

Objectives:

1. To appreciate the challenges in generating, stabilising and characterising paramagnetic compounds.
2. To understand the significance of paramagnetic species and intermediates in (bio)inorganic main group and d-block chemistry in catalysis.

3. To discuss the utility of continuous wave electron paramagnetic resonance for investigating 'open shell' species in (bio)inorganic chemistry and catalysis.
4. To survey advanced pulse electron paramagnetic resonance techniques and to understand the added value in resolving small electron-nuclear and electron-electron spin-spin interactions.

Photophysics of Coordination Compounds (E. Zysman-Colman, CH5517, 2 credits)

The aim is to provide an overview of the excited state properties of coordination compounds. This will be accomplished through detailed analysis of the photophysical behaviour of archetypal complexes such as $[\text{Ru}(\text{bpy})_3]^{2+}$. Basic concepts in photophysics and photochemistry will also be introduced.

Objectives:

1. To explain the nature of the ground and excited states in coordination compounds, the different types of transitions, understand Jablonski diagrams.
2. To understand how one measures accurately these properties: absorption spectroscopy and emission spectroscopy.
3. To understand how electroluminescent devices such as organic light-emitting diodes work and to understand how solar harvesting devices such as solar cells work.
4. To understand the nature of electron and energy transfer between separate photoactive molecules.
5. To discuss selected examples that illustrate structure/photophysical property relationships in coordination compounds.

Blockbuster Solids – Perovskites (P. Lightfoot, CH5518, 2 credits)

Aims: To build on the principles of solid state chemistry introduced in earlier modules, illustrated by examples of important contemporary solids. To understand the factors controlling the functional behaviour of complex solids in terms of solid state structure, composition and chemistry, and to have some understanding of how to design novel solids that might have a particular function.

Objectives:

1. To understand some of the important crystal structure types that occur in inorganic solid state chemistry, particularly the perovskite structure and its derivatives.
2. To understand the key compositional and structural features that control physical properties in various important families of electronically-active inorganic solids: superconductivity in cuprates, magnetoresistance in manganites and ferroelectricity in titanates, for example.
3. To appreciate the role of crystallographic symmetry in controlling certain physical properties of solids.
4. To understand how crystallographic techniques are used in the detailed characterisation of these functional materials, in particular advanced applications of X-ray and neutron powder diffraction.

Blockbuster Solids – Porous Solids (R. Morris, CH5518, 2 credits)

Aims: To build on the principles of solid state chemistry introduced in earlier modules, illustrated by examples of important contemporary solids. To understand the factors controlling the functional behaviour of complex solids in terms of solid state structure, composition and chemistry, and to have some understanding of how to design novel solids that might have a particular function.

Objectives:

1. To understand how porous solids are important for many different chemical applications.
2. To develop an understanding of how the structure of porous solids is important for applications in ion exchange, catalysis, separations and medicine.
3. To appreciate how the scale and size of pores affects features such as transport and storage properties.
4. To understand how modern porous materials have the potential to impact many areas in the future, and how the chemistry of the porous materials is vital to full realisation of new solids.

Enzyme co-factors (D. O'Hagan, CH5612, 2 credits)

Aims: To appreciate the origin of natural products and the diversity of enzyme reactions. In depth understanding of the role of co-factors at the mechanistic level, allowing a general understanding of metabolic processes and how we can study them..

Objectives:

1. General discussion of enzyme co-factors.
2. NADH/NADPH and flavins (FAD/FADH₂) and other enzymes.
3. Pyridoxal 5'-phosphate (PLP) enzymes concentrating on their importance in amino acid metabolism including decarboxylation, racemisation and transamination.
4. Thiamin pyrophosphate (TPP) enzymes.
5. Co-enzyme B12 dependent enzymes.

Biosynthesis (T. K. Smith, CH5612, 2 credits)

Aims: To appreciate the origin of natural products and the diversity of enzyme reactions. In depth understanding of the role of co-factors at the mechanistic level, allowing a general understanding of metabolic processes and how we can study them.

1. How do we study biosynthesis- in vivo and in vitro?
2. Metabolic Pathways- "The power house" Glycolysis and the Krebs cycle.
3. Fatty acid and lipid biosynthesis.
4. The Mevalonate and non-mevalonate pathways- leading to polyisoprenoid (terpenes and steroid) biosynthesis.
5. Putting knowledge into practice- enzyme assays and high throughput screening.

Natural products (G. Florence, CH5612, 2 credits)

Aims: To appreciate the origin of natural products and the diversity of enzyme reactions. In depth understanding of the role of co-factors at the mechanistic level, allowing a general understanding of metabolic processes and how we can study them.

1. The structure and biosynthesis of common plant alkaloids from amino acid building blocks will be covered including the tropane and morphine families of natural products and related alkaloids.
2. The origin of diversity of aliphatic and aromatic polyketide structures, and use of labeled acetate precursors, to follow polyketide biosynthesis.
3. The biosynthesis of aromatic polyketides from 6-methylsalicylic acid to daunamycin will be reviewed starting from acetate as a building block.

Reactive intermediates (R. A. Aitken, I. A. Smellie, CH5613, 3 credits)

Aims: To develop a broad understanding of the chemistry of key types of reactive intermediates including carbenes, nitrenes, arynes, carbocations and radicals. To understand how they can be generated, detected and characterised. To review how each type of reactive intermediate can be used in the synthesis of organic compounds including natural products.

Objectives:

1. To introduce general and specific methods for generating and detecting each type of reactive intermediate.
2. To study the most important reactions of carbenes and nitrenes i.e. insertion, cycloaddition and rearrangement.
3. To review inter- and intra-molecular reactions of arynes with nucleophiles and in cycloadditions.
4. To understand the use of flash vacuum pyrolysis in the generation of reactive intermediates in the gas phase.
5. To understand contemporary applications of carbenes, nitrenes and arynes and carbocations in synthesis.
6. To review the key reactions of carbocations.
7. To understand the key reactions of free radicals i.e. chain reactions incorporating addition, abstraction, electron transfer, rearrangement, cyclisation, homolytic substitution and termination steps. To review annulation and ring enlargement processes.
8. To review cascade reactions of free radicals, particularly multiple cyclisations and cyclisation/translocation/fragmentation combinations. To examine cascades involving radical addition to unsaturated molecules and subsequent (or prior) cyclisation steps.

Chemical Biology (N. J. Westwood, CH5614, 2 credits)

The aim of this course is to introduce and discuss modern approaches in chemical biology and drug development. The multidisciplinary nature of the process will be emphasised and several examples of recent successes will be covered. A balance of subjects at the interface of chemistry and biology will be discussed. This course will be suitable for anyone with an interest in applied organic chemistry and/or drug discovery and/or methods in chemical biology.

Objectives:

1. An overview of chemical biology and its synergistic relationship with drug discovery.
2. Examples of the use of chemical tools to study biological processes.
3. Approaches used in the discovery of chemical tools including the essential roles of protein crystallography, screening methods, fragment-based methods and chemical library generation from a range of sources.
4. Challenges associated with the discovery and use of chemical tools: Issues raised will include protein specificity, target identification and successfully mining chemical space.
5. Contrasting the properties of chemical tools with compounds of importance in medicinal chemistry and drug discovery.
6. Examples of drug discovery projects including state of the art applications recently published by industry in anti-cancer, antibacterial, anti-viral and anti-parasitic drug discovery.
7. Other research topics within the provided definition of chemical biology will be discussed in detail with a specific literature example being given in each case.

Molecular recognition (D. Philp, E. R. Kay, CH5616, 3 credits)

The principal aim of this course is to introduce the student to the processes involved in the non-covalent interactions of molecules in solution. It will provide a fundamental understanding of intermolecular interactions and introduce the fundamental concepts and processes of molecular recognition in solution. The course will provide the basis for the characterisation, quantification, and analysis of molecular associations and illustrate how this knowledge can be applied to understand small molecule–small molecule associations and to engineer specific molecular recognition interactions.

The course will illustrate and expand on these principles through a series of short case studies from the recent literature.

Objectives:

1. To understand the basic definitions of host–guest chemistry and supramolecular chemistry.
2. To understand the basic principles of molecular interaction thermodynamics in solution, and the fundamental electrostatic interaction: pole–pole, pole–dipole, dipole–dipole, dispersion.
3. To recognise of hydrogen bonds and understand the features determining their strength, directionality and origins.
4. To be able to encode and decode patterns of hydrogen bonds and appreciate the role and importance of secondary interactions.
5. To recognise the strength, directionality and origins of interactions between π -systems and between π -systems and cations.
6. To recognise the strength and origins of the hydrophobic effect.
7. To understand the basic principles involved in thermodynamic description of intermolecular binding phenomena, and an awareness of experimental methods that may be used to measure these experimentally.
8. To appreciate how features including molecularity and cooperativity affect binding phenomena.
9. To appreciate the basic principles required for selective molecular recognition, including complementarity and preorganization.
10. To appreciate the design, binding affinities and binding selectivity of crown ethers and other ion–dipole recognition systems.
11. To appreciate the design, binding affinities and binding selectivity of cyclodextrins.
12. To appreciate the design, binding affinities and binding selectivity of cyclophanes.
13. To appreciate the design, binding affinities and binding selectivity of molecular clefts.
14. To appreciate the application of design principles to create selective molecular recognition systems for neutral molecules using hydrogen bonds.
15. To appreciate the design and function of supramolecular catalysts.
16. To appreciate the role of self-assembly in the construction of large ordered molecular and supramolecular assemblies in the natural and unnatural world.
17. To understand the principles of self-assembly of unnatural systems.
18. To understand the principles of template-assisted synthetic strategies for the construction of macrocyclic and interlocked molecular structures.
19. To appreciate how covalent bond formation under thermodynamic control may be combined with noncovalent interactions to drive selection from dynamic combinatorial libraries and to facilitate the efficient template-assisted construction of complex molecular architectures.
20. To appreciate the use of environmental stimuli to modify host-guest interactions and understand the design and operation of simple molecular switches and molecular machines.
21. To be aware of the experimental methods which are useful in determining the presence and strength of molecular associations, and understand the application of these methods for characterizing supramolecular systems.

Surface science (C. J. Baddeley, CH5713, 2 credits)

To introduce the main techniques of surface science and to understand how these techniques can be used to investigate the structure, composition and reactivity of surfaces with a particular focus on systems of relevance to heterogeneous catalysis.

Objectives:

1. To introduce the concepts of order and roughness when describing solid surfaces. The concept of and nomenclature associated with two dimensional crystallinity will be discussed.
2. To introduce the concepts of adsorption and desorption.
3. To introduce techniques for the characterization of solid surfaces – e.g. low energy electron diffraction and scanning probe microscopy.
4. To introduce methods of elemental analysis at surfaces.
5. To introduce techniques for the characterisation of molecular adsorbates at surfaces – e.g. surface vibrational spectroscopies.

Heterogeneous catalysis (P. Wright, CH5713, 10 lectures, 2 credits)

To introduce the important general concepts of the chemistry of heterogeneous catalysis and to describe and illustrate the main types. To derive the mechanism of catalytic reactions from experimental data.

1. To understand the role of a catalyst in relation to thermodynamics and to appreciate the relevance of catalyst activity, selectivity, deactivation and regeneration.
2. To identify the major types of heterogeneous catalysts (metals, metal oxides and solid acids) and be familiar with the general principles of their mode of action.
3. To interpret kinetic data of catalytic reactions in terms of adsorption equilibria and elemental reaction steps and to be familiar with the Langmuir-Hinshelwood and Eley-Rideal kinetic models.
4. To develop the concept of an active site in heterogeneous catalysis and to apply physical techniques in characterising the catalytic centres.
5. To understand the application of chemical techniques, such as isotopic labelling and product composition, to elucidate reaction mechanism. To examine case histories of important and topical catalytic reactions, e.g.:
6. To know the catalytic action of supported metals and in particular the platinum group metals, for example in automobile catalytic converters
7. To understand the catalytic action of solid acids, including zeolites, and the use of bifunctional catalysts.
8. To be aware of new developments of catalysis over microporous solids, including selective oxidation
9. To be aware of new developments of catalysis over nanoparticulate gold.

Chemical Applications of Electronic Structure Calculations (J. Mitchell, M. Buehl, CH5714, 3 credits)

The course will build on the foundations laid in the modules CH2701 and (CH3712) and discuss further aspects and methods of modern computational chemistry related to the electronic structures of atoms and molecules. It will be shown how results of such calculations can be used to complement, interpret, and guide experiments in many areas of chemistry.

Objectives:

1. To provide an overview of ab initio methods and their associated "model chemistries".
2. To discuss density functional theory and give an overview of its current state-of-the-art.
3. To consider applications of computed structures and energies in chemistry.

4. To discuss both the theoretical underpinnings and the applications of molecular dynamics simulations.
5. To give an overview of the theory of intermolecular forces.
6. To discuss the development of force fields and their applications in molecular simulations.

Energy Conversion and Storage (J. T. S. Irvine, R. T. Baker, A. R. Armstrong, CH5715, 3 credits)

The aim of the course is to familiarise students with electrochemical processes occurring in the solid state. The basic mechanisms and principles of ionic conduction in solids and the electrochemical processes occurring at the interfaces of solid-state electrochemical systems will be discussed. The course will cover important technologies in energy conversion and storage in detail, including lithium ion batteries and fuel cells. Operating principles, materials requirements, advantages and disadvantages will be discussed. The course will be given in three parts: 1. Fundamental Electrochemistry (JTSI); 2. Fuel Cell Technology (RTB) and 3. Energy Storage and Batteries (ARA).

Objectives:

1. To understand the fundamentals of electrochemistry in the solid state.
2. To compare ionic conductivity in solids with that in molten salts and conventional liquid electrolytes.
3. Ionic conductivity in polymers -polymer electrolytes: what are they and how can we understand their unique mechanism of conduction?
4. To understand electrochemical processes and the application of Impedance Spectroscopy.
5. To be able to explain the general principles of fuel cells in detail and to be familiar with the main fuel cell types, their operation, advantages, disadvantages and potential applications.
6. To be able to describe and explain the operation of SOFC and PEMFC fuel cells in detail including the roles and requirements of the anode, cathode and electrolyte and the associated materials considerations.
7. To understand the energy and efficiency considerations and potential for alternative fuels in fuel cell systems.
8. To understand the mechanism of intercalation and the factors allowing a material to act as an intercalation host, to be familiar with intercalation compounds.
9. To understand the important parameters of batteries, the most common/important types and why novel ionic conductors and intercalation compounds are important for advanced batteries with particular relation to lithium-ion batteries.
10. To understand alternative mechanisms for electrode materials including alloying and conversion and their advantages and disadvantages, to be able to compare the emerging types of battery and their strengths and weaknesses and be familiar with lithium-sulfur, lithium-air and sodium-ion batteries and their possible application.

Transferable skills training

PhD Thesis Writing Workshop (EaStCHEM wide course for chemists): (a single day course to be held at the University of Edinburgh, Semester 2, transport provided, 1 credit, recommended for 3rd year PG students).

This course provides advice and information on how to write a thesis and prepare for the examination process. The session will include practical, interactive activities and contributions from experienced PhD supervisors and examiners and recent PhD graduates. Content will include:

- The role of the thesis and doctoral regulations
- The external examiner's perspective and responsibilities
- Organisation, motivation and planning
- What makes a good thesis
- Anticipating the viva

This EASTCHEM course will be held at Edinburgh. Student participants will be drawn from the EASTCHEM/SCOTCHEM partner universities of St Andrews, Edinburgh and Heriot Watt. The course will be followed by a small drinks reception hosted by EASTCHEM.

Academic Paper Writing (EaStCHEM wide course for chemists): (a single day course to be held in St Andrews in Semester 2, 1 credit)

Publishing a paper in a journal is the main and most important way of communicating the results of your research to the research community. This course offers advice and guidance on how to write a paper and get it published, from notebooks to the first draft, submission, referees' comments, publication and all the steps in between. The session will include practical, interactive activities and contributions from experienced academic authors, journal referees and journal editors. It is particularly relevant for Chemistry PhD students who are about to write, or are writing a paper for publication. Course content will include:

- Understanding journal ratings and impact factors
- Preparing the paper: journal formats and submission
- The Editorial process – what are reviewers looking for
- Responding for reviews; resubmission of the revised manuscript.