ScotCHEM
Everything that Matters

ScotCHEM Module Catalogue
2019-20

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Contents

*** The credit scores listed are those awarded at the modules' home institutions and are not transferable between ScotCHEM schools/departments. We provide these details for information only. Your own school/department will decide how many credits it is appropriate to award. Please contact your local Graduate Studies Coordinator for advice.**

NB: When you take an online module for credit, unless we tell you otherwise, the assessment will take place at the same time as for the physical class. This might mean that you have access to the module content well in advance of the assessment.

SEMESTER 1

Interfacial Electrochemistry

Lecturer	Institution
Dr A. Cuesta	Aberdeen

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
ABN1	15	10	1	10.19

Description

Aims

To introduce the students to current models of (i) the interface between a metal or a semiconductor and an electrolyte, (ii) interfacial electron transfer, and (iii) the kinetics and mechanism of electrochemical reactions, as well as to the experimental methods for their study. The technological relevance of this knowledge in areas as different as energy conversion and storage, metal plating and corrosion, and surface micro- and nanostructuring will be emphasized.

Learning Outcomes

At the end of this course you should be able to:

- Understand the concepts of the electrical double layer, surface charge density, and interfacial capacitance.
- Relate fundamental concepts of Surface Science to those of Interfacial Electrochemistry.
- Explain the Butler-Volmer equation.
- Understand the concepts of overpotential, exchange current density and Tafel slope.
- Understand semiconductor electrochemistry and photoelectrochemistry.
- Obtain kinetic information from cyclic voltammograms, chronoamperograms and rotating disk electrode polarization curves.
- Describe the challenges associated to the development of electrochemical energy storage and conversion devices.

Synopsis

1. The electrode - electrolyte interface.
    - The electrical double layer.
    - The capacitance of the electrode electrolyte interface, the potential of zero charge of metal electrodes, and the flat band potential of semiconductor electrodes.
    - Comparing the metal-ultrahigh vacuum and metal-electrolyte interfaces.
    - Technological relevance: supercapacitors, electrowetting and electrolenses.
2. Interfacial electron transfer.
    - Empirical models: Tafel equation and Butler-Volmer equation.
3. The mechanism and kinetics of electrochemical reactions.
    - Electrochemical kinetics and electrocatalyisis
    - The importance of the surface atomic structure in electrocatalysis
    - Technological relevance: fuel cells
4. Methods
    - Electrochemical methods
    - In situ non---electrochemical methods

Reading

W. Schmickler and E. Santos, *Interfacial Electrochemistry*, Springer, 2010.

J.O'M. Bockris, A.K.N. Reddy and M. Gamboa---Aldeco, *Modern electrochemistry. Volume 2A, Fundamentals of electrodics*, Kluwer, 2002.
A.J. Bard and L.R. Faulkner , *Electrochemical methods: fundamentals and applications*, John Wiley, 2000.

Assessment

Short Essay or answering a set of 2 – 3 questions as homework

Magnets, Metals and Superconductors

Lecturer	Institution
Dr A. McLaughlin	Aberdeen

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
ABN2	15	10	1	09.19

Description

Aims

To introduce the phenomenon of magnetism observed in discrete molecular clusters and solid state transition metal oxides. Interesting electronic properties such as superconductivity and colossal magnetoresistance observed in the layered cuprates, arsenides and manganites respectively will also be described.

- Understand magnetism associated with isolated magnetic ions, molecular clusters and transition metal oxides.
- Predict the effective magnetic moment.
- Explain the quenching of orbital angular momentum, which occurs extensively in first row transition metal ions.
- Describe the different types of magnetic ordering such as ferromagnetism, antiferromagnetism and ferrimagnetism.
- Predict the type of magnetic order observed by considering kinetic and potential superexchange pathways.
- Understand the concept of spin frustration.
- Understand the magnetic order, which occurs in metallic oxides.
- Describe the phenomena of high temperature superconductivity and colossal magnetoresistance.

Synopsis

1) Single ions and polynuclear complexes
   - Magnetic susceptibility
   - Differences between theoretical and experimental values of the effective magnetic of lanthanide free ions.
   - Differences between theoretical and experimental values of the effective magnetic of first row transition metal free ions.
   - Magnetic Exchange interactions
   - Spin frustration
2) Magnetism and conductivity in transition metal oxides
   - Transition metal oxide structure types.
   - Magnetic order in insulating oxides.

- Superconductivity.
- Magnetoresistance

Reading
Solid State Chemistry and its Applications (2nd edition), A. R. West, Wiley, 2014.
Transition metal oxides: structure, properties and synthesis of ceramic oxides, *C. N. R. Rao and B. Raveau,* Wiley-- VCH, 1998.
High temperature superconductivity: an introduction, *G. Burns*, Academic, 1992.

Assessment

Short Essay

Research and Research Ethics

Lecturer	Institution
Dr A. Cuesta	Aberdeen

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
ABN3		10	1	09.19

Description

These are not regular lectures, rather Aberdeen has shared its printed materials, so that students from other institutions can prepare essays and referee mock papers. Aberdeen will then provide feedback.

The description below is taken from the Aberdeen student handbook:

The course consist of a series of discussions in which students are introduced to how research functions at present. This include an introduction to how research is conducted and funded, how the public and other scientists are informed about results from the research, and the peer-review process. The relevance of research ethics and integrity, as well as the development of an ethical code of practice for research are considered and discussed throughout the course. The assessment is based (i) on analysis of real examples of potentially non-ethical research behaviour and its impact on the wider community; (ii) an exercise of refereeing a manuscript potentially intended for submission to a scientific journal.

Assessment

Short Essay analysing an ethical case study, refereeing a research article

Environmentally Significant Materials

Lecturer	Institution
Dr A. McCue	Aberdeen

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
ABN5	5	10	1	09.19

Description

Aims:
To provide an understanding of the concept of *risk* in the treatment of contaminated land and to introduce functional materials and their use in remediation and waste management.
Learning Outcomes:
At the end of this course you should be able to:

- Explain the concept of risk and recognise the principal components of risk assessment
- Critically compare and select optimum remediation strategies for particular types of contaminated sites
- Explain the principles of the multi-barrier concept for waste immobilisation
- Apply risk assessment criteria to the treatment of hazardous wastes

Synopsis:
1) Risk Assessment and Land Remediation

- Definitions of risk and risk assessment
- Legislative guidelines on contaminated land
- Remediation strategies

2) Environmentally Significant Materials in Waste Management

- Nuclear fuel cycle and waste reprocessing
- Cement matrices for radioactive wastes
- Cements and contaminated land
- Clays and zeolites in waste management
- Photocatalysis and related processes – oxidative degradation of organic pollutants.

3) Oil spills

- Oil composition and basic properties
- How these properties change after a spill
- Methods for remediating an oil spill

Reading Material:

- ‘Environmental Chemistry; a global perspective’, GW van Loon and SJ Duffy (Oxford, 2005).
- ‘Environmental Chemistry’, 2nd Ed., C Baird, (Freeman, 1999).
- ‘The Basics of Oil Spill Cleanup’, 3rd Ed., M FIngas (CRC Press, 2012).

Assessment
Short Essay

Practical Computational Chemistry

Lecturer	Institution
Dr H. Fruchtl	St Andrews

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
STA1	2	10	1	10.19

Description

Course Summary
The course will introduce practical computational chemistry techniques. The focus is on the current state-of-the-art computational chemistry codes together with the theory behind the methods. Ab initio, DFT and classical methods, as well as cheminformatics, will be introduced along with how they are used in practice by researchers in Scotland.

Course Description
The course starts with a short introduction to the theoretical foundations of most of quantum chemistry, including Hartree-Fock, post-HF methods, Density Functional Theory and the principles of Cheminformatics. One lecture will cover High Performance Computing and Linux. Visualisation of molecules and their properties will be followed by a more practical introduction into calculations on molecules and periodic materials. Example inputs for Gaussian (molecular quantum chemistry) and CASTEP (periodic DFT) are discussed. Assessment is via assignments. For the practical assignments a remotely accessible computer cluster and the necessary software is provided.
Learning Outcomes
- Understand the main theories used in computational chemistry and cheminformatics
- Use Linux and a queuing system to edit files and run calculations.
- Use several software packages to calculate, optimise and visualise geometries and other properties of molecules and materials.

Reading list
"Introduction to Computational Chemistry" by Frank Jensen
"Materials Modelling using Density Functional Theory: Properties and Predictions" by Feliciano Guistino
"Machine learning methods in chemoinformatics", J.B.O. Mitchell,
WIREs Comput. Mol. Sci., 4, 468-481 (2014)

Assessment

Continuous assessment.

An Introduction to Asymmetric Synthesis

Lecturer	**Institution**
Prof A. Smith	St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
STA7	2	10	1	09.19

Description

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 stoicheiometric 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.

Assessment

Open book exam.

Reactor Engineering

Lecturer	**Institution**
Prof S. Roy	Strathclyde

ModuleID	**Credits**	**Teaching Hours**	**Semester / Session**	**Start Date**
STR4	10	18	1	09.19

Description

This module demands a good understanding of the underlying mathematics.

Educational Aim

This module aims to introduce the students to the principles of chemical reactors and reactor design across a range of chemical engineering contexts, as a first and fundamental course in reactors. From fundamentals of energy and mass balance the course proceeds in increasing complexity of reactor design and performance. The course also aims to bring about an appreciation and judgement of how to optimise for single and multiple reactions as well as the effect of multiple reactors for increased capacity and performance.

Learning Outcomes

On completion of the module the student is expected to be able to

LO1 Understand the basis of chemical reactor design in terms of mass balances, kinetics, energy balances and stoichiometry.

LO2 Performance equations for different types of reactors – batch, flow – continuous stirred tank and plug flow reactors

LO3 Know how to take into account multiple reactions (parallel and series reactions) operating series in the design and analysis of reactors.

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(UK SPEC suggests no more than 4 learning outcomes per module. Statements must be broad and be syllabus free and link in with the intended learning outcomes on the programme specifications.)

Syllabus

The module will cover the following topics:

(i) Chemical equilibria and the role of equilibria in designing reactors (and controlling reactions)
(ii) reaction kinetics and complex reactions such as reversible, series and parallel reactions, rate limiting step
(iii) stoichiometry and its role in understanding limiting reactant and conversion
(iv) Ideal reactors - batch, plug flow and continuous stirred tank reactors
(v) Design considerations for single reactors/reactions, operating points and considerations for optimisation
(vi) Design of multiple reactors, continuous reactors with recycle, and reactors in series,
(vi) Design consideration for multiple reactions – series and parallel reactions, selectivity and yield as performance indicators

Assessment of Learning Outcomes

For each of the Module Learning Outcomes the following criteria will be used to make judgements on student learning:

LO1 Understand the basis of chemical reactor design in terms of mass balances, kinetics, energy balances and stoichiometry.
C1 Write the design equations for different reactor types and apply them to gas phase and liquid phase reactions for reactor sizing or determining conversion.

LO2 Performance equations for different types of reactors – batch, flow – continuous stirred tank and plug flow reactors
C2 Use design equations to size reactors, estimate capacity and optimise for different kinetics.

LO2 Know how to take into account multiple reactions (parallel and series reactions), in the design and analysis of reactors.
C3 Use reaction kinetics and design equations to obtain product distributions in competing reactions

LO3 Know how to take into account multiple reactors operating series in the design and analysis of reactors.

C4 Extend mass balances to size reactors or determine conversions when multiple reactors are operated in series and parallel. Estimate how to increase capacity of a process by doing so.

Assessment

Exam

SEMESTER 2

Registration for these modules will not open until January.

Biomaterials

Lecturer	Institution
Prof. I. R. Gibson	Aberdeen

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
ABN4	15	10	2	13.01.20

Description

Aims:
This course aims to introduce the concept of biomedical materials, and the role of materials chemistry in their design and performance.

Required Prior Knowledge:
This general course will require knowledge drawn from various lower level courses, in particular from solid-state chemistry and in general materials chemistry.

Learning Outcomes
Students completing this course should be able to:

- Apply fundamental aspects of physical and materials chemistry, such as electrochemistry, phase diagrams, and spectroscopy to the synthesis of biomaterials;
- Understand and discuss the implications of mechanical and biological properties when synthesising a new biomaterial;
- Describe how the surface of a bioceramic implant will respond to a physiological environment;
- Discuss how chemical modification of current implant materials may enhance their biological performance.
-

Synopsis

- Ceramics and glasses – the advantages and disadvantages of using these materials to produce implants. In particular, the properties of mechanical strength vs. biological response will be compared.
- Coatings, in particular ceramic coatings on metallic implants
- Polymers – a comparison of the expected properties of polymers to be used as implants including mechanical strength, biodegradation, and biofouling.
- Surface properties of materials, including surface charge, contact angle, microstructure.
- Biological interaction with material surfaces – how proteins and cells interact with the surface of biomaterials.
-

Suggested Reading (not required to purchase)
Biomaterials, Sujata V. Bhat. Boston; London, Kluwer Academic Publishers, 2002. Library: 610.28 Bha.
Biomaterials science: An introduction to materials in medicine, edited by Buddy D. Ratner - Amsterdam; London, Academic Press, 1996. Library: 610.28 Rat.
Biomaterials : An introduction, Joon Bu Park and Roderic S. Lakes. New York, Plenum Press, c1992. Library: 610.28 Par2

An introduction to bioceramics, editors, Larry L. Hench & June Wilson. -- Singapore; London, World Scientific, 1993. Library: 610.28 Hen
Bioceramics: Materials, properties, applications, Antonio Ravaglioli and A. Krajewski ; -- London; New York, Chapman & Hall, 1991. Library: 666 Rov.

Assessment

Electrochemistry for a Sustainable Future

Lecturer	**Institution**
Dr M. Symes	Glasgow

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
GLA2	1	8	2	27.01.20

Description

Aims:

This course will examine the applications of electrochemistry in a variety of contexts of relevance to sustainable chemical processes. We shall investigate electrochemical methods for water purification, metal extraction and energy (harvesting, storage and conversion). Many of the examples shown are at the cutting edge of scientific and technological research. The emphasis throughout the course will be on the interplay between fundamental concepts and the materials required to perform the tasks of interest.
No previous knowledge of electrochemistry is assumed: all the concepts we will require to describe the relevant systems will be explained during the course.

Intended Learning Outcomes

Lecture 1: Introduction to Electrochemistry. After this lecture you should be familiar with the concepts of electrochemical potential and basic electrochemical processes such as bulk electrolysis and cyclic voltammetry.
Lecture 2: Fuel Cells. After this lecture you should be familiar with the concepts of the fuel cell and be able to explain how fuel cells work and which material properties are desirable when designing such devices.
Lecture 3: Electrolysis of Water. After this lecture you should understand why electrolytic production of hydrogen from water is important and be able to compare different methods of electrolysis and different materials for this purpose.
Lecture 4: Batteries. After this lecture you should be able to describe, explain and evaluate the concepts behind and performance of a selection of battery technologies, including lead-acid batteries, Li-ion batteries and redox flow batteries.
Lecture 5: Photo-electrochemistry. After this lecture you should understand what a photoelectrochemical cell is and how it works in terms of its materials of construction, and be able to assess the relative performance of different cells.

Lecture 6: Water Purification. After this lecture you should be able to explain the various electrochemical methods of water purification and be able to give a reasoned account of their various merits and demerits.
Lecture 7: Metal Extraction. By the end of this lecture you should be able to explain the different electrochemical strategies used to obtain metals from their ores and be able to assess these in terms of their relative efficiency and environmental impact.
Lecture 8: Electrochemical Fuel Production. In this final lecture we will examine current research in the direct synthesis of fuels using electrochemistry, looking in particular at the electrochemical reduction of CO_2. We will use the skills and knowledge acquired during the previous seven lectures to assess the prospects for this avenue of research.

Suggested Reading:
1. Electrochemical Methods: Fundamentals and Applications, 2nd Edition Allen J. Bard and Larry Faulkner (John Wiley and Sons, 2001).
2. Materials for a Sustainable Future, Trevor M. Letcher and Janet L. Scott (Eds.) (RSC Publishing, 2012).

Assessment

Exam

Advanced Physical Instrumentation Techniques

Lecturer	**Institution**
Dr S Greaves, Dr N. Nahler	Heriot Watt

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
HWT1	15	20	2	01.19

Description

Aims:
This module aims to present an advanced discussion of some important topics in modern Physical Chemistry:
- Instrumental Control, Data Acquisition and Processing
- Principles of Light, Optics and Lasers
- Applications of Laser Based Measurements
- Principles of Interfacial Measurements

Learning Outcomes:
On completion of this module, the learner will be able to demonstrate:
• Demonstrate detailed knowledge and understanding of applied physical chemistry, at the forefront of the subject
• Display a critical understanding of the concepts, theories and principles discussed in the module • Integrate previous knowledge from across chemistry with the topics discussed in the module
• Analyse, evaluate and interpret new methods and techniques at the forefront of chemistry
• Execute a defined literature research project and identify applications to specific tasks

• Use fundamental principles to solve both qualitative and quantitative analytical problems
• Apply specialised skill to the solution of some chemical problems

The module provides the opportunity to :
• Critically review and consolidate knowledge, skills and practices in chemistry
• Communicate with professional level colleagues through diverse modes such as presentations, posters and news articles
• Interpret and evaluate a wide range of information to solve problems of both a familiar and unfamiliar nature
• Use a range of software to support and enhance work at an advanced level
• Manage time effectively, work to deadlines and prioritise workloads
• Use ICT skills with on-line materials to support the learning process
• Apply strategies for appropriate selection of relevant information from a wide source and large body of knowledge
• Exercise initiative and independence in carrying out literature research and learning activities

Syllabus:
• Instrumental Control, Data Acquisition and Processing: Introduction to the concepts and practice of experimental data acquisition and control, data analysis methods. Using photonic and particle detectors as example sources of signals
• Principles of Optics and Lasers: Fundamental nature of light, introduction to optics, refraction, diffraction and interference effects. Principles of lasers, mode-locking, chirped pulse amplification, practical laser systems, commercially available lasers, linear and non-linear optical response, SHG, SFG, third order effects, wave mixing energy level diagrams, external optical cavities.
• Application of Laser Based Measurements: Modern high resolution spectroscopic techniques, LIF and REMPI. Laser absorption, including cavity enhanced and modulation techniques, limits of detection. Application to laboratory studies of kinetics and trace chemical analysis. Principles of time resolved optical experiments, wavepackets, Transient absorption and femtosecond Raman techniques

Assessment

Poster presentation.

Advanced NMR Problems

Lecturer	**Institution**
Dr T. Lebl	St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
STA2	2	6	2	05.20

Description

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.

Assessment

Continuous assessment.

An Introduction to Fortran

Lecturer	**Institution**
Dr T. van Mourik	St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
STA3	2	20	2	03.20

Description

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. No prior programming experience is required.

Assessment

Continuous assessment.

Crystallography

Lecturer	**Institution**
Prof P. Lightfoot	St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
STA4	2	6	2	05.20

Description

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.

Assessment

Continuous assessment.

Electron Microscopy

Lecturer	Institution
Prof W. Zhou	St Andrews

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
STA5	2	6-8	2	05.20

Description

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.

Assessment

Assignment

Solid State NMR

Lecturer	Institution
Prof S. Ashbrook	St Andrews

ModuleID	Credits*	Teaching Hours	Semester / Session	Start Date
STA6	2	10	2	03.20

Description

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.

Assessment

Open book exam.

The 'Antibiotic Apocalypse' – what can chemists do about it?

Lecturer	Institution
Prof Colin Suckling	Strathclyde

ModuleID	Credits	Teaching Hours	Semester / Session	Start Date
STR1	2	5-6	n/a	04.20

Description

Everyone, even politicians, agree that we need new antibiotics to combat resistant strains of infectious organism. Resistance is not a new problem; it has been around since the first antibiotics were introduced but the scale of the problem is now global and critical. Every infectious agent, bacteria, viruses, fungi, and parasites, shows resistance to existing treatments. It's not a remote problem either; Scottish hospitals struggle to find successful treatments for some bacterial infections. As one of the primary sources of new medicines, chemistry and chemists can make a strong contribution to providing new and effective anti-infective medicines. This course will review the history of anti-infective drugs and resistance to them leading to more detailed discussions of modern efforts to obtain new antibiotics to treat the wide range of infectious diseases that afflict humans and animals. A basic knowledge of cell biology (DNA, protein biosynthesis etc.) at a general science level will be required and further relevant biology will be presented in the course. The chemical content will include compound design, molecular modelling, synthesis, and mechanism of action studies.

Assessment

A short written assignment

High resolution NMR spectroscopy for small molecules

Lecturer	Institution
Dr John Parkinson	Strathclyde

ModuleID	Credits	Teaching Hours	Semester / Session	Start Date
STR2	2	1	2	03.20

Description

The course describes NMR methods that are used for determining structures of small molecules in solution. While the emphasis is placed on small organic molecule applications, the principles are transferable.

This is primarily a web-based course which includes on-line problem solving exercises and worked examples. An introductory lecture will be given where general information and the web link for the course material will be provided.

Assessment

A problem solving exercise at the end of the set period for viewing the course material

The practice and pitfalls of studying organic reaction mechanisms

Lecturer	Institution
Dr Marc Reid	Strathclyde

ModuleID	Credits	Teaching Hours	Semester / Session	Start Date
STR3	2	5-6	2	Summer

Description

Outline:
Mechanism matters. From small academic laboratories to industrial pilot plants, the study of reaction mechanisms is vital for controlling and predicting the outcome of a chemical process. In this class, we revisit concepts in kinetics introduced at undergraduate level, and consider how we can avoid the most common mistakes when trying to understand linear and catalytic reactions in more depth.

Learning Outcomes:
1) Understand the concepts of reaction order, molecularity, and elementary steps.
2) Understand the difference between 'Steady State' and 'Pre-equilibrium' approximations.
3) Understand the importance of analysing reaction at different temperatures and the mechanistic information this provides.
4) Understand the fundamentals of linear free energy relationships and their various applications in mechanistic analyses (e.g. the Hammett relationship).
5) Understand the applications of isotopes in studying reaction
6) Understand the differences in studying linear *versus* catalytic reactions.

Assessment

Written assignment based on unseen examples of mechanistic experiments

REVIEW ONLY

Computational Chemistry and Modelling; Electronic Structure Theory and Classical Simulation Methods

Lecturer	**Institution**
	Edinburgh and St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
EDNSTA1	n/a	25	Online	Online

Description

We provide the series of three computational chemistry modules EDNSTA2-4 on an audit only basis *i.e.* there is no assessment.

The modules provide a more in-depth look at the material covered in SUPACCH Practical Computational Chemistry. You can use them either, as an alternative to, or a study aid for SUPACCH.

Assessment

Audit Only

Computational Chemistry and Modelling; Computational Modelling of Materials

Lecturer	**Institution**
	Edinburgh and St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
EDNSTA2	n/a	25	Online	Online

Description

We provide the series of three computational chemistry modules EDNSTA1-3 on an audit only basis *i.e.* there is no assessment.

The modules provide a more in-depth look at the material covered in SUPACCH Practical Computational Chemistry. You can use them either, as an alternative to, or a study aid for SUPACCH.

Assessment

Audit Only

Computational Chemistry and Modelling; Computer Aided Drug Design

Lecturer	**Institution**
	Edinburgh and St Andrews

ModuleID	**Credits***	**Teaching Hours**	**Semester / Session**	**Start Date**
EDNSTA3	n/a	25	Online	Online

Description

We provide the series of three computational chemistry modules EDNSTA2-4 on an audit only basis *i.e.* there is no assessment.

The modules provide a more in-depth look at the material covered in SUPACCH Practical Computational Chemistry. You can use them either, as an alternative to, or a study aid for SUPACCH.

Assessment

Audit Only

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