# ScotCHEM Module Catalogue

# 2017-18

| | |
|---|---|
| Author: | Dr S.J. Lilley |
| Approved: | |
| Document Number: | SC180715 |
| Version: | 2.5 |
| Release Date: | |
| Printed: | 21.12.2017 |

# Interfacial Electrochemistry

| Lecturer | Institution |
|---|---|
| Dr A. Cuesta | Aberdeen |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| ABN1 | 5 | 10 | 1 | 15.10.17 |

**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.
   - Differences between theoretical and experimental values of the effective magnetic of first row transition metal free ions.
   - 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

# Magnets, Metals and Superconductors

| Lecturer | Institution |
|---|---|
| Dr A. McLaughlin | Aberdeen |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| ABN2 | 5 | 10 | 1 | 13.09.17 |

**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 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.
- Explain the mean field theory of ferromagnetism and antiferromagnetism.
- 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 and structural distortions
2) Magnetism and conductivity in transition metal oxides
   - Transition metal oxide structure types.
   - Mean field theory of ferromagnetism and antiferromagnetism.
   - Magnetic order in metallic oxides.

- Colossal magnetoresistance in La1---xSrxMnO3 perovskites.
- Superconductivity.

**Reading**

J. S. Miller and A. J. Epstein, *Angewandte Chemie. Int. Ed. English.* 33, 385---415 (1994).
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

# Chemistry of the f-block

| Lecturer | Institution |
|---|---|
| Dr D Price | Glasgow |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| GLA1 | 5 | 8 | 1 | 20.11.17 |

**Description**

**Aims:**

The chemistry of the f-block elements is introduced. The course will examine both chemical and physical properties of these elements and their compounds, with an emphasis on the relationship between properties and underlying electronic structure.

**Intended Learning Outcomes**

By the end of this lecture block students will be able to:

1. Recall of the names, symbol and position in the periodic table of f-block elements
2. Describe the shape and extent of 4f and 5f orbitals.
3. Explain the origin of the lanthanide contraction.
4. Describe coordination geometries of lanthanide and actinide ions.
5. Describe trends in redox chemistry in the f-block elements
6. Describe and explain the differences and similarities between the chemistry of the lanthanides, the actinides and the d-block transition metal elements.
7. Understand the limitations of Russell-Saunders and j-j coupling schemes and the influence of relativistic effects in describing the electronic structures of these elements.
8. Correlate electronic, magnetic and optical properties with the electronic structures of the 4f elements.
9. Describe the uses of lanthanides and actinides in the nuclear industry.
10. To assess the likely decay mechanisms for given actinide isotopes.
11. Describe the basic chemistry of more stable actinides: Thorium to Americium.

**Outline:**

- Occurrence, isolation and current applications of lanthanide elements;
- The nature of f-orbitals, and the electronic structures of lanthanide atoms and ions;

- The lanthanide contraction and coordination chemistry (including coordination numbers and stereochemistry);
- Properties of the elements and binary compounds;
- Electronic properties of lanthanides, coupling schemes and electronic and magnetic materials;
- Spectral properties of lanthanides, and optical materials;
- Occurrence and discovery (and synthesis) of the actinides;
- Nuclear properties of actinides; isotope stability and decay mechanisms;
- Lanthanides and actinides in the nuclear industry:
- Reaction chemistry of actinides.

**Recommended Reading:**
Inorganic Chemistry and Atkins, Overton, Rourke, Weller, Armstrong, OUP, 5th Edition, 2010. Advanced Inorganic Chemistry, F A Cotton and G Wilkinson, John Wiley, 6th Edition. Chemistry of the Elements, N N Greenwood and A Earnshaw, Pergamon, 2nd Edition.

**Assessment**

Exam

# Advanced Physical Instrumentation Techniques

| Lecturer | Institution |
|---|---|
| Dr S Greaves, Dr N. Nahler | Heriot Watt |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| HWT1 | 5 | 20 | 2 | xx.01.18 |

**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. |

# Computational Chemistry and Modelling – Electronic Structure Theory and Classical Simulation Methods

| **Lecturer** | **Institution** |
| --- | --- |
| | Edinburgh and St Andrews |

| **ModuleID** | **Level** | **Teaching Hours** | **Semester / Session** | **Start Date** |
| --- | --- | --- | --- | --- |
| EDNSTA1 | 6 | 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** | **Level** | **Teaching Hours** | **Semester / Session** | **Start Date** |
|---|---|---|---|---|
| EDNSTA2 | 6 | 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** | **Level** | **Teaching Hours** | **Semester / Session** | **Start Date** |
|---|---|---|---|---|
| EDNSTA3 | 6 | 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

# Practical Computational Chemistry

| Lecturer | Institution |
|---|---|
| Dr H. Fruchtl | St Andrews |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| STA1 | 6 | 10 | 1 | 20.09.17 |

**Description**

**Course Summary**
The course will provide an introduction to practical computational chemistry techniques. The focus is on an introduction to 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.

# Advanced NMR Problems

| Lecturer | Institution |
|---|---|
| Dr T. Lebl | St Andrews |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| STA2 | 6 | 6 | 2 | May |

**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** | **Level** | **Teaching Hours** | **Semester / Session** | **Start Date** |
|---|---|---|---|---|
| STA3 | 6 | 20 | 2 | TBC |

**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** | **Level** | **Teaching Hours** | **Semester / Session** | **Start Date** |
|---|---|---|---|---|
| STA4 | 6 | 6 | 2 | TBC |

**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 | Level | Teaching Hours | Semester / Session | Start Date |
| --- | --- | --- | --- | --- |
| STA5 | 6 | 6-8 | 2 | TBC |

**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**

Continuous assessment.

---

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

| Lecturer | Institution |
| --- | --- |
| Prof Colin Suckling | Strathclyde |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
| --- | --- | --- | --- | --- |
| STR1 | 6 | 5-6 | tbc | tbc |

**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.

Delivered via the SMSTC Vscene video conferencing facility.

**Assessment**

Probably a short written assignment

# High resolution NMR spectroscopy for small molecules

| Lecturer | Institution |
|---|---|
| Dr John Parkinson | Strathclyde |

| ModuleID | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| STR2 | 6 | 1 | Summer | Summer |

**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.

Delivered via the SMSTC Vscene video conferencing facility.

**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 | Level | Teaching Hours | Semester / Session | Start Date |
|---|---|---|---|---|
| STR3 | 6 | 5-6 | Summer | 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.

Delivered via the SMSTC Vscene video conferencing facility.

**Assessment**

Written assignment based on unseen examples of mechanistic experiments