# CH3F1-15 Advanced Physical Chemistry and Laboratory

## 22/23

**Department**
: Chemistry

**Level**
: Undergraduate Level 3

**Module leader**
: Phillip Stansfeld

**Credit value**
: 15

**Module duration**
: 6 weeks

**Assessment**
: 33% coursework, 67% exam

**Study location**
: University of Warwick main campus, Coventry

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## Description

## Introductory description

N/A

Module web page

## Module aims

This module provides an introduction to two advanced topics in physical chemistry; interfacial chemistry and molecular modelling.

First, this module will develop students' knowledge of the properties of surfaces and interfaces, and the methods available for characterising them. Here, students will be introduced to the physical chemistry of a range of surface and interfacial processes, including both solid and liquid interfaces, as well as experimental methods for characteristing surfaces, ranging from scanned probe microscopy (including atomic force microscopy, scanning tunnelling microscopy and electrochemical microscopy) to spectroscopic methods. A significant aspect of this module is to demonstrate the importance of surfaces processes in chemistry and the borders of chemical engineering, biomedical science, materials science and physics.

Second, students will be introduced to basic concepts in molecular modelling, focussing on molecular dynamics simulations using empirical force-fields. Starting from the Born-Oppenheimer approximation, this part of the module will cover the basics of molecular dynamics simulations, including periodic boundaries, integration algorithms, and implementation of different thermodynamic ensembles. As well as providing a firm grounding in the theoretical basis of molecular dynamics simulations, this module will also emphasize what properties can be calculated, and the connection between molecular dynamics and statistical mechanics.

As well as standard lectures, these aims will be supported by experimental laboratory sessions which have an emphasis on designing and implementing experiments. In a similar manner, the theoretical and computational aspects of this course will be supported by workshops sessions with an emphasis on giving practical experience of running classical molecular simulations.

## Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

Surfaces and interfacial chemistry:

1. Introduction. Scope of surface and interfacial chemistry. Examples.
2. Solid surfaces. Structures and indexing of single crystal surfaces. Miller indices. Kossel model of surfaces: steps, terraces, kink sites, defects. Screw dislocations.
3. Scanning tunnelling microscopy (STM). Principles of tunnelling. Dependence of tunnelling current on distance and barrier height. Constant current vs. constant height modes. Applications of STM.
4. Atomic force microscopy (AFM). Principles and instrumentation. Features in tip-approach curves. Contact, non-contact and tapping (intermittent contact) modes. In situ AFM studies of crystal growth and dissolution. Surface charge measurements and testing DLVO theory with AFM measurement.
5. Chemically and electrochemically sensitive SPM techniques. Chemical force microscopy (CFM). Scanning electrochemical microscopy (SECM)-AFM. Scanning ion conductance microscopy (SICM). Scanning Electrochemical Cell Microscopy (SECCM).
6. Adsorption on solids and chemically-functionalised surfaces. Langmuir adsorption isotherm. Self-Assembled Monolayers and applications.
7. Photoelectron spectroscopy (XPS) and surface spectroscopy.
8. Fractal surfaces. Fractal geometry of surfaces. Determination of fractal dimensions of a surface. Implications for surface area measurements. Contact angle measurements.
9. Liquid surfaces. (double topic) Surface tension. Soap bubbles. Young-Laplace equation. Effects of various solutes on surface tension. Surfactants and surface pressure. Gibbs adsorption isotherm and applications.
10. Monolayer films and bilayer membranes. Langmuir film balance and applications. Isotherms. Characterisation of monolayers by fluorescence microscopy. FRAP and lateral diffusion.

Molecular modelling:

1. General concepts in molecular modelling. Coordinate systems, hardware and software.
2. Empirical force-fields and interatomic potentials. Born-Oppenheimer approximation.

Discussion of typical empirical force-fields, including functional forms and parameterization strategies. Periodic boundary conditions.
3. Molecular dynamics. Introduction to molecular dynamics method, discussion of molecular dynamics as a route to calculating dynamic and thermodynamic properties of molecules and materials. Connection with statistical mechanics.
4. Modelling applied to problems in surface and interface chemistry.
5. Examples of molecular modelling studies. What can and cannot be calculated using molecular dynamics simulations with empirical force-fields?
6. Application of molecular modelling and AI to solve protein structure prediction.
7. Use of molecular modelling for virtual screening of small molecule interactions.

## Learning outcomes

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

- Index simple crystal surfaces using Miller indices
- Understand the importance and scope of interfacial chemistry.
- Understand in basic terms what a contact angle on a solid surface indicates
- Have an appreciation for classical aspects of the subject, including liquid surfaces, surfactants and monolayer films.
- Appreciate the types of defects that are commonly found on solid surfaces and their consequences for reactivity
- Understand the principles and some of the applications of common surface spectroscopic methods
- Understand the principles of STM (tunnelling)
- Appreciate the applications of STM to surface structure, adsorption, and atomic manipulation.
- Understand the principles of AFM
- Describe fundamental methods and approximations in molecular modelling and molecular dynamics simulations
- Describe typical empirical force-fields and interatomic potentials for modelling interactions between atoms and molecules in condensed-phase environments and compare their abilities/limitations.
- Analyse a given chemical problem to decide whether the problem is amenable to molecular modelling and, if so, design a suitable computational protocol.
- Apply computational chemistry techniques to illustrative problems, analyse the results and critically interpret their significance.
- Understand the connection between molecular dynamics simulations and classical statistical mechanics.
- Be aware of the types of properties which can and cannot be calculated in classical molecular dynamics simulations with empirical force-fields.
- Be able to design a physical chemistry experiment making use of information from scientific literature
- Appreciate how molecular modelling and artificial intelligence can be used to predict macromolecular structures
- Understand how scanned electrochemical probes work and where they can be used

- Understand the basis and use of common adsorption isotherms such as Gibbs adsorption and Langmuir adsorption
- Understand how fluorescence recovery after photobleaching works and what it can be used to measure
- Understand the basis for the Young-Laplace equation and its modern applications

## Indicative reading list

Parts of the chapters entitled "Materials 1: macromolecules and aggregates", "Materials 2: the solid state" and "Processes at solid surfaces" in Physical Chemistry, Peter Atkins and Julio de Paula, OUP (Chs 19, 20 and 25, in 8th edition) provides reasonably good coverage of some aspects of the course.

More specialised texts include:
"Modern Techniques of Surface Science", D.P. Woodruff (Cambridge, 2016)
"Solid Surfaces, Interfaces and Thin Films", H. Lüth (Springer, 2010)
"Surface Science Techniques", G. Bracco and H. Bodil eds. (Springer, 2010)

“Physical Chemistry of Surfaces", A.W. Adamson (Wiley, 5th or 6th edition).
“Surface Science: Foundations of Catalysis and Nanoscience” Kurt W. Kolasinski, 2002, Wiley, 2nd edition
“Colloid and Surface Chemistry", D. J. Shaw (Butterworth, 3rd or 4th edition).
There are numerous papers and resources on the web that will help with parts of the course. These are given to students in lectures to emphasise particular aspects and updated each year.

Computational Chemistry. J. Harvey (Oxford Chemistry Primers 2018)
Molecular Modelling: Principles and Applications, 2nd Edition. A. Leach (Pearson 2001)
Essentials of computational chemistry, C. J. Cramer (Wiley 2005)
Understanding molecular simulation, D. Frenkel and B. Smit (Academic press 2002)
Molecular quantum mechanics, P. W. Atkins and R. S. Freedman (Oxford 2001)

## Subject specific skills

Numeracy
Problem solving
Critical thinking
Organisation and time management

## Transferable skills

Numeracy
Problem solving
Critical thinking
Organisation and time management

## Study

## Study time

| Type | Required |
| --- | --- |
| Lectures | 21 sessions of 1 hour (14%) |
| Practical classes | 5 sessions of 6 hours (20%) |
| Other activity | 6 hours (4%) |
| Private study | 93 hours (62%) |
| Total | 150 hours |

## Private study description

N/A

### Other activity description

Other activities cover:

1. Problem based workshop (one for each half of the course)
2. Question and answer session (one for each half of the course)
3. Revision workshop (one for each half of the course)

## Costs

No further costs have been identified for this module.

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## Assessment

You do not need to pass all assessment components to pass the module.

Students can register for this module without taking any assessment.

### Assessment group D3

| Assessment component | Weighting | Study time | Eligible for self-certification |
| --- | --- | --- | --- |
| Laboratory Report | 33% | | Yes (extension) |

| | Weighting | Study time | Eligible for self-certification |
|---|---|---|---|
| Reassessment component is the same | | | |
| **Assessment component** | | | |
| In-person Examination | 67% | | No |

- Answerbook Pink (12 page)
- Students may use a calculator
- Periodic Tables
- Graph paper

**Reassessment component is the same**

### Feedback on assessment

Cohort level examination feedback provided via Moodle. Written feedback on laboratory report from assessor.

Past exam papers for CH3F1

## Availability

### Pre-requisites

To take this module, you must have passed:

- All of
  - CH162-30 Introduction to Physical Chemistry
  - CH273-15 Properties of Solutions and Foundations of Electrochemistry and Statistical Mechanics
  - CH274-15 Electrons in Molecules and Solids

### Post-requisite modules

If you pass this module, you can take:

- CH412-15 Advanced Biophysical Chemistry
- CH406-15 Electrochemistry and Nanotechnology
- CH413-15 Advanced Computational Chemistry
- CH401-60 Research Project & Methodology

## Courses

This module is Core for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
    - Year 4 of F101 Chemistry (with Intercalated Year)
    - Year 4 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
    - Year 3 of F100 Chemistry
    - Year 3 of F121 Chemistry with Medicinal Chemistry
- Year 3 of UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
- Year 4 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-4M Undergraduate Master of Chemistry Variants
    - Year 3 of F100 Chemistry
    - Year 3 of F105 Chemistry
    - Year 3 of F125 MChem Chemistry with Medicinal Chemistry
- Year 4 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)