CH3F1-15 Advanced Physical Chemistry and Laboratory

20/21

Department
Chemistry
Level
Undergraduate Level 3
Module leader
Giovanni Costantini
Credit value
15
Module duration
6 weeks
Assessment
33% coursework, 67% exam
Study location
University of Warwick main campus, Coventry

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 such as atomic force microscopy and scanning tunnelling microscopy. 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, Schottky and Frenkel defects. Screw dislocations. Growth modes of solid surfaces (Frank-van der Merwe; Stranski-Krastanov; Volmer-Weber). Comparison of site reactivities.
3. Surface spectroscopy. Photoelectron spectroscopy (XPS and UPS). Surface infra-red spectroscopy.
4. Scanning tunnelling microscopy (STM). Principles of tunnelling. Dependence of tunnelling current on distance and barrier height. Vertical and lateral resolution: constant current vs. constant height modes. Dependence on voltage, scanning tunnelling spectroscopy (STS).
5. Applications of STM. Examples of atomic-level STM images: surface structure, images and registry of adsorbed molecules. STM of metals, semiconductors and molecular adsorbates. Time-resolved STM. Wavefunction mapping. STM-induced manipulation: writing with atoms.
6. Atomic force microscopy (AFM). Principles and instrumentation. Features in tip-approach curves. Contact, non-contact and tapping (intermittent contact) modes. Q-plus AFM. Application of AFM: imaging, probing, manipulating.
7. New generation STM techniques. Scanning ion-conductance microscopy (SICM). Scanning electrochemical microscopy (SECM). Combined SECM-AFM. Scanning near-field optical microscopy (SNOM).
8. Fractal surfaces. Fractal geometry of surfaces. Determination of fractal dimensions of surface. Implications for surface area measurements. Contact angle measurements.
9. Liquid surfaces. Surface tension. Effects of various solutes on surface tension. Surfactants. Soap bubbles. Young-Laplace equation. Surface pressure. Gibbs adsorption isotherm.
10. Monolayer films and bilyaer membranes. Langmuir film balance and applications. Isotherms for gaseous, condensed and expanded films. Characterisation of monolayers by fluorescence microscopy. Lateral diffusion in monolayers. Diffusion across cell membranes.
11. Chemially-functionalised surfaces. Langmuir-Blodgett films and applications. Self-assembled monolayers and films.
12. Surface reactions and kinetics (1). Steps in a surface reaction. Crystal growth and

dissolution.
13. Surface reaction and kinetic (2). Electrode reactions and electrocatalysis.

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?

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, reactivity and 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

Indicative reading list

The chapter entitled "Processes at solid surfaces" in Physical Chemistry, Peter Atkins and Julio de Paula, OUP (Ch 28, in 7th edition) provides reasonably good coverage of several aspects of the course.
More specialised texts include
“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).
“Surfaces and Interfaces of Solids”, H. Lueth (Springer Series in Surface Sciences - Vol. 15, Springer Verlag, 1993)
There are numerous papers that will help with parts of the course. These are given to students in lectures to emphasise particular aspects and updated each year.

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	5 hours (3%)
Total	150 hours

Type	Required
Private study	94 hours (63%)
Total	150 hours

Private study description

N/A

Other activity description

Workshops

Costs

No further costs have been identified for this module.

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 D1

	Weighting	Study time
Laboratory Report	33%	
In Person Examination	67%	

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
- CH413-15 Advanced Computational Chemistry
- CH412-30 Advanced Biophysical Chemistry
- CH401-60 Research Project & Methodology
- CH406-15 Electrochemistry and Nanotechnology

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 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)