CH3H3-15 Predictive Chemical Modelling

26/27

Department
Chemistry
Level
Undergraduate Level 3
Module leader
Scott Habershon
Credit value
15
Module duration
5 weeks
Assessment
20% coursework, 80% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

This module builds on concepts covered in Year 1 and Year 2 modules and expands knowledge and understanding of molecular simulations, electronic structure calculations and machine learning. The module includes numerous “case studies” to both diversify the content and highlight the usefulness of computational chemistry in research contexts and industrial scenarios.

Module web page

Module aims

By the end of the module students should gain understanding of the foundations underpinning the main methods used in modern computational chemistry, be able to choose appropriate methods to address specific computational modelling problems and to assess their capabilities and limitations.

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.

The module is split into 3 topics that will be delivered via lectures and supported by workshops. Each section will also cover applications and case studies.

1. Electronic structure calculations
2. Machine learning
3. Molecular simulations

Learning outcomes

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

- Demonstrate understanding of the theoretical foundations underpinning the main methods used in modern computational chemistry, including molecular dynamics, electronic structure theory, and machine learning methods.
- Choose appropriate methods to address specific computational modelling problems from various modern application areas.
- Apply computational chemistry methods to calculate measurable molecular and materials properties and analyse the results of simulations.
- Assess the capabilities and limitations of common computational chemistry tools and their relationship to experimental techniques.
- Design and create modelling, simulation, and visualisation workflows via scientific coding and machine learning techniques.

Indicative reading list

Reading lists can be found in Talis

Specific reading list for the module

Subject specific skills

Thermodynamics
Kinetics
Spectroscopy and Characterisation

Transferable skills

Problem Solving
Digital Literacy
Mathematics

Study

Study time

Type	Required
Lectures	20 sessions of 1 hour (13%)
Practical classes	5 sessions of 1 hour (3%)
Private study	125 hours (83%)
Total	150 hours

Private study description

N/A

Costs

No further costs have been identified for this module.

Assessment

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

Assessment group D

	Weighting	Study time	Eligible for self-certification
Assessment component			
Essay based on discussion with expert researcher	20%		Yes (extension)

A guest lecture will be held, delivered by an expert in one of the aspects of computational chemistry covered in this module. The lecture will describe a contemporary piece of research in computational chemistry, and will include time for discussion and student questions. Students will then be tasked with writing a short summary of the class discussion, focusing on which frontier chemistry challenges the methods described could address and how.

Reassessment component is the same

Assessment component			
Centrally-timetabled examination (On-campus)	80%		No

Written Examination

	Weighting	Study time	Eligible for self-certification

- 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 following the Exam Board.

Past exam papers for CH3H3

Availability

Courses

This module is Optional 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 4 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 3 of F109 MChem Chemistry (with International Placement)
  - Year 3 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - 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)