CH3F4-15 Molecular Structure and Dynamics

24/25

Department
Chemistry
Level
Undergraduate Level 3
Module leader
Scott Habershon
Credit value
15
Module duration
10 weeks
Assessment
25% coursework, 75% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

N/A

Module web page

Module aims

Quantum mechanics is the basis for the understanding of many chemical phenomena including photochemistry and spectroscopy. Building on the elementary concepts introduced over the first two years, this module develops more rigorously the tools needed to understand how the electronic structure of molecules is computed and how advanced quantum mechanical concepts and state-of-the-art experimental methodologies are used to study various aspects of chemical dynamics, from electronically excited states to chemical reaction rates.

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.

Electronic Structure Calculations: Introduction to MO theory, Variational principle, Hartree-Fock theory, Configuration Interaction and other past-Hartree-Fock methods, Excited state wavefunctions, Density Functional Theory, Calculating properties of chemical structures and reactions using electronic structure methods.

Electronic Spectroscopy: Born-Oppenheimer approximation and vibronic levels. Franck-Condon principle. Absorption and emission.

Photophysics & Photochemistry: General introduction to photochemistry, light absorption and electronically-excited states, the physical deactivation of excited states, radiative processes of excited states, intramolecular radiationless transitions of excited states, lasers and exemplar literature as discussion papers.

Learning outcomes

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

- Recognise the fundamental role of the variational principle in chemistry and its application to the computation of electronic structure of molecules.
- Describe how quantum chemical calculations can be used to investigate chemical reactions by, for example, calculating energy barriers and reaction rates
- Describe the advantages and disadvantages of different quantum chemical methods and their role in the interpretation of the experiment.
- Understand the nature of the states probed by electronic spectroscopy of molecules and the processes of radiative and non-radiative relaxations following excitation.
- Describe the difference between the reactivity in the ground and the excited molecular states and characterizing the different types of photochemical processes.
- Discuss contemporary research in chemistry based on electronic structure calculations and ultrafast spectroscopy and explore how these methods could be used as the basis of novel research projects.

Indicative reading list

A.R. Leach, Molecular Modelling, Principles and Applications
C. Cramer, Essentials of computational chemistry
G.H. Grant & W.G. Richards, Computational Chemistry
P. W. Atkins, Molecular Quantum Mechanics
N.J. Turro, Modern Molecular Photochemistry

Subject specific skills

Numeracy
Problem solving
Oral communication

Transferable skills

Numeracy

Problem solving
Oral communication

Study

Study time

Type	Required
Lectures	20 sessions of 1 hour (12%)
Seminars	10 sessions of 1 hour (6%)
Practical classes	4 sessions of 1 hour (2%)
Other activity	40 hours (25%)
Private study	76 hours (47%)
Assessment	12 hours (7%)
Total	162 hours

Private study description

76 hrs of revision and self-study

Other activity description

10 hrs completing workshop exercises
10 hrs ideas pitch preparation
20 hrs directed reading

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 D8

	Weighting	Study time
Computer Workshop Problems	15%	

Students will use modern computational methods to investigate the properties (e.g. structure,

	Weighting	Study time

vibrations) of molecular systems, and investigate the properties of chemical reactions.

Idea pitch	10%	12 hours

In small groups, students will take part in developing a scientific research idea that uses or develops concepts related to the content of this module. These ideas will then be pitched to the rest of the cohort; assessment will be based on an individual presentation the student's proposal.

Molecular Structure and Dynamics	75%

Feedback on assessment

Formal feedback to be provided for the computer workshop, the assessed presentations and the written abstracts of guest lectures. Cohort level examination feedback provided via Moodle.

Past exam papers for CH3F4

Availability

Courses

This module is Optional for:

- 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 F109 MChem Chemistry (with International Placement)
  - Year 3 of F126 MChem Chemistry with Med Chem (with Prof Exp)
  - Year 3 of F125 MChem Chemistry with Medicinal Chemistry
  - Year 3 of F106 MChem Chemistry with Professional Experience
- Year 4 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)

This module is Option list A 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 3 of UCHA-4M Undergraduate Master of Chemistry Variants