UNSW Course Outline

CHEM3011 Quantum Nature of Molecules - 2024

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General Course Information

Course Code : CHEM3011
Year : 2024
Term : Term 3
Teaching Period : T3
Is a multi-term course? : No
Faculty : Faculty of Science
Academic Unit : School of Chemistry
Delivery Mode : In Person
Delivery Format : Standard
Delivery Location : Kensington
Campus : Sydney
Study Level : Undergraduate
Units of Credit : 6

Useful Links

Handbook Class Timetable

Course Details & Outcomes

Course Description

This course builds on previous physical chemistry content and deepens students' understanding and ability to utilise contemporary computational and experimental methods to solve chemical problems. It will explore the phenomenological nature of matter at the quantum scale.

The course focuses on establishing the theoretical foundations and introducing powerful techniques including symmetry, quantum chemistry, and statistical thermodynamics. The use of modern experimental tools to obtain accurate molecular energies, spectra and thermodynamic data is also described.
Throughout the course, there will be an emphasis on applications of these techniques, for example, in atmospheric chemistry, catalysis and material science.
CHEM3011 is taught as a combination of lectures, workshops and laboratory classes with written assignments and laboratory reports assessed throughout the session.

Course Aims

The aim of this course is to prepare students for research activities in the use of physical and computational techniques to predict molecular behaviour and reaction outcomes that are crucial in many areas of chemistry. The course aims to develop the understanding of the students in these areas:

- Theory of Molecular Energy
- Modern Quantum Chemical Methods
- Modern Experimental Methods

The broad aims of the laboratory and workshop programs are to:

- illustrate and reinforce aspects of the lecture program
- provide students with opportunities to acquire and practice the basic skills of practical physical chemistry: namely acquiring, interpreting and analysing various types of data and
- provide students with the opportunity to acquire the essential skills of contemporary computational chemistry.

Course Learning Outcomes

Course Learning Outcomes
CLO1 : Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.
CLO2 : Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.
CLO3 : Describe the extension of quantum mechanical methods to periodic solid state and heterogeneous systems.
CLO4 : Apply statistical thermodynamics to describe the link between atomic and molecular energies and chemical equilibria and kinetics.
CLO5 : Perform calculations of molecular properties and reaction mechanisms using contemporary computational chemistry packages.

Course Learning Outcomes	Assessment Item
CLO1 : Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.	• Practical Reports • Final Exam • Assignments • Mid-Term Exam
CLO2 : Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.	• Practical Reports • Final Exam • Assignments • Mid-Term Exam
CLO3 : Describe the extension of quantum mechanical methods to periodic solid state and heterogeneous systems.	• Practical Reports • Final Exam • Assignments
CLO4 : Apply statistical thermodynamics to describe the link between atomic and molecular energies and chemical equilibria and kinetics.	• Practical Reports • Final Exam • Assignments
CLO5 : Perform calculations of molecular properties and reaction mechanisms using contemporary computational chemistry packages.	• Practical Reports • Final Exam • Assignments

Learning and Teaching Technologies

Moodle - Learning Management System

Learning and Teaching in this course

The course will comprise of three hours of lectures, two hours of workshop and three hours of laboratory work per week. Hence the face-to-face teaching load will be 8 hours per week. The course will be assessed through 4 assignments issued throughout the course, laboratory reports and a mid-session and final examinations.

Assessments

Assessment Structure

Assessment Item	Weight	Relevant Dates
Practical Reports Assessment Format: Individual	30%	
Final Exam Assessment Format: Individual	40%	
Assignments Assessment Format: Individual	20%	
Mid-Term Exam Assessment Format: Individual	10%	

Assessment Details

Practical Reports

Assessment Overview

You will have hands-on experience with contemporary spectroscopic and computational techniques. You will use these techniques to measure and/or calculate equilibrium constants, molecular spectra and properties to determine structure-activity relationships and reaction outcomes. Assessment will consist of reports that will cover short answer questions, data presentation, analysis and discussion. Marks will be awarded, and feedback will be provided through comments on reports and general feedback posted on Moodle. (Weeks 1-5 and 7-9)

You will have six days to complete each lab report, and feedback will be returned in 1 week.

Each lab report carries the same assessment weighting.

Hurdle: You must attend a minimum of 7/8 laboratory classes and achieve a minimum overall score of 50% to meet the pass level requirement for the course.

Course Learning Outcomes

- CLO1 : Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.
- CLO2 : Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.
- CLO3 : Describe the extension of quantum mechanical methods to periodic solid state and heterogeneous systems.
- CLO4 : Apply statistical thermodynamics to describe the link between atomic and molecular energies and chemical equilibria and kinetics.
- CLO5 : Perform calculations of molecular properties and reaction mechanisms using contemporary computational chemistry packages.

Assignment submission Turnitin type

Not Applicable

Hurdle rules

You must attend a minimum of 7/8 laboratory classes and achieve a minimum overall score of 50% to meet the pass level requirement for the course.

Generative AI Permission Level

Simple Editing Assistance

In completing this assessment, you are permitted to use standard editing and referencing

functions in the software you use to complete your assessment. These functions are described below. You must not use any functions that generate or paraphrase passages of text or other media, whether based on your own work or not.
If your Convenor has concerns that your submission contains passages of AI-generated text or media, you may be asked to account for your work. If you are unable to satisfactorily demonstrate your understanding of your submission you may be referred to UNSW Conduct & Integrity Office for investigation for academic misconduct and possible penalties.
For more information on Generative AI and permitted use please see here.

Final Exam

Assessment Overview

The final exam is designed to summarise your learning and problem-solving skills on all topics delivered across all weeks of the term, including material from lectures, laboratories and workshops. The exam is typically 2hrs 10 minutes and consists of MCQ, short numerical and short answer responses - details will be confirmed during the course. The examination will occur during the official university examination period. Feedback is available through inquiry with the course convenor. Hurdle requirement: must achieve 35% to receive a passing grade in the course.

Course Learning Outcomes

- CLO1 : Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.
- CLO2 : Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.
- CLO3 : Describe the extension of quantum mechanical methods to periodic solid state and heterogeneous systems.
- CLO4 : Apply statistical thermodynamics to describe the link between atomic and molecular energies and chemical equilibria and kinetics.
- CLO5 : Perform calculations of molecular properties and reaction mechanisms using contemporary computational chemistry packages.

Hurdle rules

Must achieve 35% (final and mid-term exams combined) to receive a passing grade in the course.

Generative AI Permission Level

No Assistance

This assessment is designed for you to complete without the use of any generative AI. You are

not permitted to use any generative AI tools, software or service to search for or generate information or answers.
For more information on Generative AI and permitted use please see here.

Assignments

Assessment Overview

Assignments consist of quizzes and worksheets that will help you apply the content covered in the lectures to solve problems of varying difficulty. Assignments are typically due on weeks 3, 5, 8 and 10 and are worth 5% each. Feedback will be provided by way of written comments on the completed work or student-initiated meetings, within 1 week.

Course Learning Outcomes

- CLO1 : Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.
- CLO2 : Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.
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Mid-Term Exam

Assessment Overview

The midterm test is designed as a summative assessment of the learning outcomes assesses for the topics covered in weeks 1-4 inclusive (lecture material only). The midterm test will typically be scheduled in week 5 or 7 as a single attempt with a time limit of 45 minutes. The test consists of multiple-choice and short answer questions - details will be confirmed during the course. Feedback will be provided through the gradebook to link incorrect answers to topic learning outcomes and via a generalised class feedback discussion in lectures, within 1 week.

Course Learning Outcomes

- CLO1 : Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.
- CLO2 : Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.

Generative AI Permission Level

No Assistance

This assessment is designed for you to complete without the use of any generative AI. You are not permitted to use any generative AI tools, software or service to search for or generate information or answers.
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General Assessment Information

Students will gain marks in Assignments, Laboratory Reports and written Test and Exam on the basis of the correct answer. Consideration is given to follow on errors.

Guidelines as to the standards expected of Report Elements and the Final Laboratory Report are provided on Moodle.

Feedback on assessment

Selected tutorials will be used to provide general feedback on Mid-Term Test and Assignments.

The students will receive weekly feedback on their Laboratory reports from the Laboratory Demonstrators.

This feedback is intended to serve as preparation for the written examinations: Mid-Term Test

and Final Exam.

Grading Basis

Standard

Requirements to pass course

All assessment tasks, including laboratory reports, should be submitted online through the course Moodle portal. To be submitted onto Moodle by 23:59 hours on their due date unless otherwise specified. Please check Moodle for the most updated information.

Any report submitted after the due date will incur a 10% / day penalty up to 7 days, after which a mark of 0 will be awarded for that report, though feedback will still be provided if a report is submitted.

Important note: To be awarded a pass in this subject, students must satisfy four conditions:

1. An overall pass (≥ 50%) in the laboratory component,
2. A minimum attendance of 7 out of the 8 laboratory classes
3. Satisfactory overall performance (≥ 35%) in the final and mid-term examinations (combined) and
4. An overall pass (≥ 50%) for the weighted average of the assessment tasks is required.

Failure to satisfy all criteria could result in either a FL or UF (Unsatisfactory Fail) grade being awarded, or further assessment being offered at the sole discretion of the course coordinator.

Course Schedule

Teaching Week/Module	Activity Type	Content
Week 1 : 9 September - 15 September	Lecture	Group theory and symmetry
	Workshop	
	Laboratory	
Week 2 : 16 September - 22 September	Lecture	Group theory and symmetry
	Workshop	
	Laboratory	
	Assessment	Point group and symmetry assignment
Week 3 : 23 September - 29 September	Lecture	Quantum chemistry
	Workshop	
	Laboratory	
	Assessment	Point group and symmetry assignment
Week 4 : 30 September - 6 October	Lecture	Quantum chemistry
	Workshop	
	Laboratory	
Week 5 : 7 October - 13 October	Lecture	Quantum chemistry
	Workshop	
	Laboratory	
	Assessment	Mid-session exam
Week 6 : 14 October - 20 October	Other	Flexibility week - no classes.
Week 7 : 21 October - 27 October	Lecture	Statistical thermodynamics
	Workshop	
	Laboratory	
	Assessment	Quantum chemistry assignment
Week 8 : 28 October - 3 November	Lecture	Statistical thermodynamics
	Workshop	
	Laboratory	
Week 9 : 4 November - 10 November	Lecture	Periodic density functional theory
	Workshop	
	Laboratory	
	Assessment	Statistical thermodynamics assignment
Week 10 : 11 November - 17 November	Lecture	Periodic density functional theory
	Workshop	

Attendance Requirements

Students are strongly encouraged to attend all classes and review lecture recordings.

General Schedule Information

This course consists of 8 hours of class contact hours per week. You are expected to take an additional 4 hours of non-class contact hours per week to complete assessments, readings and exam preparation.

Workshops and laboratory classes are not recorded and attendance is compulsory.

Course Resources

Prescribed Resources

Physical Chemistry: Quanta, Matter and Change

Author(s): Peter Atkins, Julio de Paula and Ronald Friedman

Publisher: Oxford University Press

Year: 2014

Edition: 2nd edition

Essentials of Computational Chemistry: Theories and Models

Author(s): Christopher Cramer

Year: 2007

Publisher: Wiley

Edition: 2nd

Introduction to Computational Chemistry

Author(s): Frank Jensen

Year: 2017

Publisher: Wiley

Edition: 3rd

Density Functional Theory: A Practical Introduction

Author(s): David Scholl, Janice Steckel

Year: 2009

Publisher: Wiley

Details of additional resources will be provided on Moodle.

Course Evaluation and Development

CHEM3011 is the most advanced physical chemistry course in the School and it has been highly rated by previous cohorts for the quality of teaching.

Each year, the teaching team studies the student feedback (e.g. from MyExperience reports) and make appropriate changes to improve teaching and learning outcomes. Whilst the 2022 cohort was unanimous in their praise for the quality of teaching, they commented that there were too many assessment items due every week.

The assessment items are not overly onerous (5-10 multi choice or short answer questions in most cases) but the teaching team has acted on this feedback in 2023 by reducing~ 1/3 of the assignments and laboratory reports. This reduction is supplemented by formative assessment items such as worksheets and tutorial questions.

Staff Details

Position	Name	Email	Location	Phone	Availability	Equitable Learning Services Contact	Primary Contact
Convenor	Junming Ho				By appointment	Yes	Yes
Lecturer	Ron Haines				By appointment	No	No
	Martina Lessio				By appointment	No	No
	Timothy Schmidt					No	No

Other Useful Information

Academic Information

Upon your enrolment at UNSW, you share responsibility with us for maintaining a safe, harmonious and tolerant University environment.

You are required to:

- Comply with the University's conditions of enrolment.
- Act responsibly, ethically, safely and with integrity.
- Observe standards of equity and respect in dealing with every member of the UNSW community.

- Engage in lawful behaviour.
- Use and care for University resources in a responsible and appropriate manner.
- Maintain the University's reputation and good standing.

For more information, visit the UNSW Student Code of Conduct Website.

Academic Honesty and Plagarism

Referencing is a way of acknowledging the sources of information that you use to research your assignments. You need to provide a reference whenever you draw on someone else's words, ideas or research. Not referencing other people's work can constitute plagiarism.
Further information about referencing styles can be located at https://student.unsw.edu.au/referencing

Academic integrity is fundamental to success at university. Academic integrity can be defined as a commitment to six fundamental values in academic pursuits: honesty, trust, fairness, respect, responsibility and courage. At UNSW, this means that your work must be your own, and others' ideas should be appropriately acknowledged. If you don't follow these rules, plagiarism may be detected in your work.
Further information about academic integrity, plagiarism and the use of AI in assessments can be located at:

- The Current Students site,
- The ELISE training site, and
- The Use of AI for assessments site.

The Student Conduct and Integrity Unit provides further resources to assist you to understand your conduct obligations as a student: https://student.unsw.edu.au/conduct

Submission of Assessment Tasks

Penalty for Late Submissions

UNSW has a standard late submission penalty of:

- 5% per day,
- for all assessments where a penalty applies,
- capped at five days (120 hours) from the assessment deadline, after which a student cannot submit an assessment, and
- no permitted variation.

Any variations to the above will be explicitly stated in the Course Outline for a given course or

assessment task.

Students are expected to manage their time to meet deadlines and to request extensions as early as possible before the deadline.

Special Consideration

If circumstances prevent you from attending/completing an assessment task, you must officially apply for special consideration, usually within 3 days of the sitting date/due date. You can apply by logging onto myUNSW and following the link in the My Student Profile Tab. Medical documentation or other documentation explaining your absence must be submitted with your application. Once your application has been assessed, you will be contacted via your student email address to be advised of the official outcome and any actions that need to be taken from there. For more information about special consideration, please visit: https://student.unsw.edu.au/special-consideration

Important note: UNSW has a "fit to sit/submit" rule, which means that if you sit an exam or submit a piece of assessment, you are declaring yourself fit to do so and cannot later apply for Special Consideration. This is to ensure that if you feel unwell or are faced with significant circumstances beyond your control that affect your ability to study, you do not sit an examination or submit an assessment that does not reflect your best performance. Instead, you should apply for Special Consideration as soon as you realise you are not well enough or are otherwise unable to sit or submit an assessment.

Faculty-specific Information

Additional support for students

- The Current Students Gateway
- Student Support
- Academic Skills and Support
- Student Wellbeing, Health and Safety
- Equitable Learning Services
- UNSW IT Service Centre
- Science EDI Student Initiatives, Offerings and Guidelines

School-specific Information

UNSW Changes to Special Consideration: Short Extension

The School of Chemistry has carefully reviewed all of its assessments to determine whether they are suitable for automatic short extensions as set out by the UNSW Short Extension Policy. The current deadline structures for all assessment tasks in the School of Chemistry already accommodate the possibility of unexpected circumstances that may lead students to require additional time for submission. **The School of Chemistry has opted out of the UNSW Short Extension provision for all its courses,** and we have already integrated flexibility into our assessment deadlines. This decision is subject to revision in response to the introduction of new course offerings. All students may still apply for Special Consideration for any assessment via the usual procedures.

School Contact Information

Level 1, Dalton Building (F12)

W: www.chemistry.unsw.edu.au

Also see: ***Contacts and Support*** section of the course Moodle page (where applicable)