Course Outline

CHEM3011

Quantum Nature of Molecules

School of Chemistry

Faculty of Science

Term 3, 2021

1. Staff

Position	Name	Email	Consultation times and locations	Contact Details
Course Convenor	Junming Ho	junming.ho@unsw.edu.au	By appointment	Dalton 220
Lecturer	Ron Haines	r.haines@unsw.edu.au	By appointment	Dalton 128
Lecturer	Laura McKemmish	l.mckemmish@unsw.edu.au	By appointment	Dalton 123
Lecturer	Martina Lessio	martina.lessio@unsw.edu.au	By appointment	Dalton 124

2. Course information

Units of credit: 6

Pre-requisite(s): CHEM2011 or PHYS2111 or NANO2002

Teaching times and locations: http://www.timetable.unsw.edu.au

2.1 Course summary

Advances in computer architectures and algorithms have enabled the accurate calculation of many atomic and molecular properties. This course describes the links between molecular energies and the large-scale properties of substances such as entropy and Gibbs energies, and the rates and reaction profiles of homogeneous and heterogeneous chemical reactions. Popular computational chemistry software is introduced, with the aim of allowing students to become self-sufficient in calculating molecular properties using appropriate methods.

2.2 Course aims

CHEM3011 builds on the materials introduced in CHEM2011 and focuses on principles of group theory and symmetry, time-independent and periodic quantum chemistry, statistical thermodynamics and the practical aspects of computational chemistry. A working knowledge of these is essential for understanding all chemical reactions, including those occurring in Earth through to Space.

2.3 Course learning outcomes (CLO)

At the successful completion of this course you (the student) should be able to:

1. Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.
2. Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.
3. Describe the extension of quantum mechanical methods to periodic solid state and heterogeneous systems.

4. Apply statistical thermodynamics to describe the link between atomic and molecular energies and chemical equilibria and kinetics.
5. Perform calculations of molecular properties and reaction mechanisms using contemporary computational chemistry packages

2.4 Relationship between course and program learning outcomes and assessments

Course Learning Outcome (CLO)	LO Statement	Program Learning Outcome (PLO)	Related Tasks & Assessment
CLO 1	Assign a point group to a molecule and then use molecular symmetry to interpret vibrational spectra and other molecular properties.	Chemistry Threshold Learning Outcomes – 2.1, 2.2, 3.4, 4.2	Assignments Laboratory practicals Exams
CLO 2	Propose and apply appropriate quantum chemical methods to reliably predict molecules properties and reaction outcomes.	Chemistry Threshold Learning Outcomes – 2.1, 2.2, 3.1, 3.2, 3.3, 3.4, 4.2	Assignments Workshops Laboratory practicals Exams
CLO 3	Describe the extension of quantum mechanical methods to periodic solid state and heterogeneous systems.	Chemistry Threshold Learning Outcomes – 2.1, 2.2, 3.1, 3.2, 3.5, 3.4, 4.1	Assignments Exams
CLO 4	Apply statistical thermodynamics to describe the link between atomic and molecular energies and chemical equilibria and kinetics.	Chemistry Threshold Learning Outcomes – 2.1, 2.2, 3.1, 3.2, 3.3, 3.4, 4.2	Assignments Workshops Laboratory practicals Exams
CLO 5	Perform calculations of molecular properties and reaction mechanisms using contemporary computational chemistry packages	Chemistry Threshold Learning Outcomes – 2.1, 2.2, 3.3, 3.4, 4.2	Workshops Laboratory practicals

3. Strategies and approaches to learning

3.1 Learning and teaching activities

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.

3.2 Expectations of students

Indicate the course-specific expectations of students, including:

- Contact hours are 8 per week, in weeks 1-5 and 7-10. The major out-of-class workload is associated with the laboratory program. Pre-laboratory work is expected to take 30 minutes per week and post-laboratory write-up is expected to take 2-4 hours per week.
- Attendance at all lectures is expected and is essential for the workshop and laboratory components.
- Be fully prepared for and attend workshops and laboratory sessions
- Submission of assignments and laboratory reports by deadlines specified on Moodle.
- While data/results acquired during the lab will often be shared with a group, the student is expected to write their own independent evaluation and answers to discussion questions.
- This course is a respectful and inclusive environment in which all discourse, both within formal teaching hours and through social media is to be compliant with UNSW policies. A course-specific Q&A forum is available to all participants through the Moodle portal.

4. Course schedule and structure

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.

Week [Date/Session]	Topic [Module]	Activity [Learning opportunity]	Related CLO
Week 1	Group theory and symmetry	3 Lectures, 1 workshop, 1 lab	1
Week 2	Group theory and symmetry	3 Lectures, 1 tutorial, 1 workshop, 1 lab	1
Week 3	Quantum chemistry	3 Lectures, 1 workshop (2h), 1 lab	2, 5
Week 4	Quantum chemistry	2 Lectures, 1 lab	2, 5
Week 5	Quantum chemistry	2 Lectures, 1 workshop (2h), 1 lab	2, 5
Week 6	Flexibility week		
Week 7	Statistical thermodynamics	3 Lectures, 1 workshop (2h), 1 lab	1, 2, 4, 5
Week 8	Statistical thermodynamics	3 Lectures, 1 workshop (2h), 1 lab	1, 2, 4, 5
Week 9	Periodic density functional theory	3 Lectures, 1 workshop (2h), 1 lab	1, 2, 3, 4, 5
Week 10	Periodic density functional theory	3 Lectures, 1 workshop (2h), 1 lab	3
Week 11	Reserved for public holiday makeup classes		

5. Assessment

5.1 Assessment tasks

Assessment task	Length	Weight	Due date (indicative)[a]
Point group and symmetry assignment	No limit	5	Monday week 3 Monday week 4
Quantum chemistry assignment	No limit	5	Monday week 5 Monday week 7
Statistical thermodynamics assignment	No limit	5	Monday week 8 Monday week 9
Periodic DFT assignment	No limit	5	Friday week 10
Mid-session exam:	45 minutes	10	Wednesday week 5
Final exam:	2 hours	40	tba
Laboratory component:	3 hours x 8	30	Thursday of the subsequent week (wks. 1-5 and 7-9)

[a] To be submitted onto Moodle by 17:00 on their due date unless otherwise specified.

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

(i) An overall pass (≥ 50%) in the laboratory component,
(ii) A minimum attendance of 7 out of the 8 laboratory classes
(iii) Satisfactory overall performance (≥ 35%) in the final examination and
(iv) 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.

Further information

UNSW grading system: https://student.unsw.edu.au/grades

UNSW assessment policy: https://student.unsw.edu.au/assessment

5.2 Assessment criteria and standards

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.

5.3 Submission of assessment tasks

All assessment tasks, including laboratory reports, should be submitted online through the course Moodle portal.

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.

5.4. 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.

6. Academic integrity, referencing and plagiarism

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.[1] 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 and **plagiarism** can be located at:

- The *Current Students* site https://student.unsw.edu.au/plagiarism, and
- The *ELISE* training site http://subjectguides.library.unsw.edu.au/elise/presentation

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

[1] International Center for Academic Integrity, 'The Fundamental Values of Academic Integrity', T. Fishman (ed), Clemson University, 2013.

7. Readings and 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.

8. Administrative matters

TBA

9. Additional support for students

- The Current Students Gateway: https://student.unsw.edu.au/
- Academic Skills and Support: https://student.unsw.edu.au/skills
- Student Wellbeing, Health and Safety: https://student.unsw.edu.au/wellbeing
- Disability Support Services: https://student.unsw.edu.au/disability
- UNSW IT Service Centre: https://www.it.unsw.edu.au/students/index.html