School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

CHEM251
Foundations of Materials Science and Nanotechnology

0.1250 EFTS 15 Points
Second Semester 2024

Description

This course introduces foundational models required to predict, observe and explain the behaviour of molecules and nanomaterials.

The topics covered by this course are:
- The quantum nature of matter
- Molecular symmetry
- Transition metal chemistry

Timetable & Course Structure

Lectures and Tutorials: 4 face-to-face contact hours will be held every week. Please consult MyTimetable for lecture/tutorial times and locations.

Assignments: One assignment will be given for each topic, typically due a week after the end of each lecture block, unless otherwise notified by your lecturer. The nature of each assignment will be at the discretion of each lecturer and may take a non-traditional form, e.g. an essay or written report, a data-analysis exercise or a tutorial quiz/quizzes.

Lecturers

Assoc. Prof. Deb Crittenden: *deborah.crittenden@canterbury.ac.nz*
Assoc. Prof. Sarah Masters: *sarah.masters@canterbury.ac.nz*
Prof. Richard Hartshorn: *richard.hartshorn@canterbury.ac.nz*

Course Co-ordinator

Dr Deborah Crittenden, Department of Chemistry
Email: deborah.crittenden@canterbury.ac.nz
Contact me if you have any queries about the course.

Assessment

Each topic will contribute to the overall grade as follows:
Quantum mechanics: 25% test mark, 10% assignment grade
Molecular symmetry: 20% exam mark, 5% assignment grade
Transition metal chemistry: 30% exam mark, 10% assignment grade

This gives the following breakdown of grades by component:

End of term 3 test:	25%
End of semester exam:	50%
Assignments/tutorial work:	25%

Examination date and location details will be published on the University website. Test date and location details will be available via MyTimetable.

Textbook

P W Atkins & J de Paula, *Physical Chemistry* (8th, 9th or 10th edition). This text covers most of the material in the first two parts of this course, and is a useful supplement to the lecture material prepared by each lecturer.
C. E. Housecroft & A. G. Sharpe, *Inorganic Chemistry*, 4th Ed. This text covers the transition metal chemistry section.
Copies of both texts are available on short term loan from the Engineering and Physical Sciences Library.

Prerequisites
CHEM 211

Course Content

Introduction to quantum mechanics* (16 lecture/tutorial sessions)*: Wave-particle duality of light and matter. Introduction to the Schrodinger equation, simplifications required to make the Schrodinger solvable - model systems (particle-on-a-line, harmonic oscillator, hydrogen atom, rigid rotor), Applications of quantum models to real chemical systems, and extension to condensed phases of matter. Spectroscopy as a technique for interrogating quantum states of chemical systems – UV-Vis, infrared, microwave and photoelectron spectroscopy.

Molecular symmetry* (12 lecture/tutorial sessions)*: This part of the course will cover symmetry operations, elements and operations as well as molecular point groups and symmetry species. Symmetry considerations will be used to determine molecular polarity and chirality, analyze infrared spectra and determine orbital symmetry and bonding.

Transition metal chemistry* (20 lecture/tutorial sessions)*: Overview of concepts and definitions: Lewis acid-base concept. Classification of common ligands: donor atoms and functional groups. Multidentate and chelating ligands: stereochemistry and formation of chelate rings. Stereochemistry of metal complexes: coordination numbers 2-6 and geometry of metal complexes. Electronic structure and properties of transition metal complexes. Magnetic properties and the spin-only formula. Electronic spectra of metal complexes: UV-vis spectra; formation and stability of metal complexes. Introduction of molecular orbital theory to explain the geometries and properties of transition metal complexes.

Learning Outcomes

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

Quantum mechanics topic

- Justify each term in the Schrödinger wave equation
- Identify kinetic and potential energy terms in the Schrödinger wave equation
- Recognise solutions to the Schrödinger wave equation for simple model systems
- State how particle-in-a-box theory describes translational motion of both molecules and electrons
- Describe how the quantum harmonic oscillator model describes the vibrational motion of diatomic molecules
- Define anharmonicity, and state its importance in describing quantum nuclear motion
- Interpret how the rigid rotor model describes rotational motion
- Apply particle-in-a-box theory to predict electronic energy levels of related compounds
- Explain trends in UV-Vis spectra using the particle-in-a-box model
- Determine bond force constants of diatomic molecules, by applying the harmonic oscillator model to interpret IR spectra
- Calculate molecular moments of inertia and bond lengths, using the rigid rotor model to analyse microwave spectra
- Relate molecular orbital energy levels (occupied, unoccupied) to continuum states of solids (valence band, conduction band)
- Sketch band structures for conductors, semi-conductors and insulators
- Define the terms p-doping and n-doping, and sketch the associated electronic energy levels
- Explain how silicon photovoltaic solar panels work

Molecular symmetry topic

- Recognise and describe the symmetry elements and operations of a molecule, including the identity, rotations, reflections, rotations, improper rotations and inversion;
- Define the term similarity in the context of symmetry and be able to determine whether or not two symmetry operations are similar;
- Define, and determine the presence of, a principal axis of symmetry;

- Define the group-theoretical term point group;
- Describe, and differentiate between, point groups that are categorised as linear, uniaxial, cubic, centrosymmetric and spherical;
- Determine the point group of a molecule from its symmetry elements (or operations) and vice versa;
- Determine, from its symmetry or point group, whether a molecule is chiral and/or polar;
- Define the group-theoretical terms character and character table;
- Determine the symmetry species of molecular orbitals including those derived from the d orbitals of a transition-metal ion in an octahedral complex;
- Determine the symmetry species of the vibrations of simple molecules;
- Describe examples of the use of vibrational spectroscopy (IR and Raman) to determine the symmetry of molecules.

Transition metal chemistry topic

- Explain why the study of transition metal complexes is important and its relevance to biology, industry, and the world around us.
- Define what a transition metal complex is; be familiar with the concepts and definitions and the Lewis acid-base concept.
- Classify common ligand types, know what donor atoms and functional groups are and be able to identify what constitutes multidentate and chelating ligands; their stereochemistry and the formation of chelate rings.
- Define what coordination numbers are and know common coordination numbers 2-6 and the geometries of metal complexes they form; know what square planar, tetrahedral; trigonal bipyramid; square-based pyramid; octahedral geometries are and any common distortions associated with these geometries.
- Define what constitutes the electronic structure and properties of transition metal complexes; be able to compare and contrast ionic and covalent bonding models; be able to apply the crystal field theory to obtain the energy level diagrams in square planar; tetrahedral; trigonal bipyramid; square-based pyramid; octahedral; cubic; and pentagonal bipyramid fields etc.
- Know the consequences and applications of orbital splitting and how this affects the electronic configurations of metal complexes; be able to calculate crystal field stabilization energies (CFSE); be able to use these approaches to explain the origin of the Jahn-Teller effect; know what high-spin and low-spin configurations are and how these affect the magnetic properties of TM complexes and be able to apply the spin-only formula.
- Apply a qualitative molecular orbital theory approach to produce orbital diagrams for octahedral complexes.
- Elucidate the physical basis that gives rise to electronic spectra of metal complexes, and identify what transitions give rise to UV-visible Spectra.
- Interpret UV-visible data in the context of the Laporte and spin selection rules, extinction coefficients, and possible charge transfer transitions.
- Describe and explain the origins of the spectrochemical series.
- Critically discuss the crystal field theory and molecular orbital theory approaches in the context of explaining the spectrochemical series (π-acidic and π-basic ligands).
- Predict the formation and stability associated with TM complexes; and know how to measure and explain TM complex formation and dissociation constants; cumulative stability constants and trends; the 'chelate effect'; factors affecting stability.

GENERAL INFORMATION | TE KIMI MŌHIOHIO 2024

Policy on 'Dishonest Practice'| Ngā Takahitanga me ngā Tinihanga

The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit, a department may choose to not mark such work – see the online guidelines in relation to '[Academic Integrity]'.

The School of Physical and Chemical Sciences upholds this policy. It considers plagiarism, collusion, copying and ghost writing – all detailed below – to be unacceptable and dishonest practices:

- ***Plagiarism | Tārua Whānako*** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source. Note that the use of **AI generative tools such as ChatGPT** for assessment work is *strictly forbidden*, except where the lecturer concerned has specifically granted approval.
- ***Collusion*** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and

incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.

- ***Copying*** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) – data analysis and interpretation of obtained results MUST be performed individually.**
- ***Ghost writing*** is the use of other person(s) (whether with or without payment) to prepare all or part of an item of work submitted for assessment.

Special consideration of assessment | Ngā Pairuri Motuhake
'Special Consideration' for an item of assessment is for students who have covered the work involved but have been prevented from demonstrating their knowledge or skills at the time of the assessment due to unforeseen circumstances, whether illness, injury, bereavement, car crash or any other extenuating circumstance *beyond one's control*. Special Consideration for a test/exam may be because a student has not sat it or has done so with impaired performance. Applications can be submitted via the above link and must be made **no later than five working days after the assessment due date**. Note that special consideration is **not available for items worth less than 10% of the overall course mark**. In the case of illness or injury, medical consultation should normally have taken place either shortly before or within 24 hours after the due date for the required work or test/examination.

Note that you may be required to sit a special exam or your grade may not be changed if there is insufficient evidence of your performance from other invigilated assessment items in the course. ***You have the right to appeal any decision.***

It is important to understand that Special Consideration is only available *where course work has been covered*, and the inability to demonstrate this fully is both *no longer possible* AND is due to *unexpected circumstances beyond one's control*. Thus Special Consideration **is NOT available for:**

- essays, assignments or quizzes where an extension of time is available to complete the assessment item (see below for the process to involved);
- missed lectures during the semester;
- experiencing examination anxiety;
- having several examinations or assessments close together;
- known impairment, such as chronic illness (medical or psychological), injury or disability unless medical evidence confirms that the circumstances were exacerbated, despite appropriate management, at the time of assessment;
- mistaking the date or time of an examination (this is a circumstance one can control!);
- failing to turn up to an examination or test because of sleeping in (a circumstance as above!);
- where applications are repeatedly made for the same or similar reason, then the application may be declined on the grounds that the reason is not unexpected;
- where the application is made at the time of the assessment but the supporting documentation is received significantly after this date or after the date results are released; or
- the application is made following the release of results (unless under exceptional circumstances).

Extensions of deadlines | Tononga Wā Āpiti
Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator and/or the lecturer concerned.

Late withdrawal from a course
If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. Applications must be submitted ***within five days*** of the end of the main examination period for the semester.

Missing of tests | Te Matangaro i ngā Whakamātautau
In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams
Past tests can be found on our Chemistry Undergraduate website. Past exams can be found on the Library website.

Submission of reports and assignments
Reports (including lab reports) and assignments should be handed in on time. Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.

Note: If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

Late Work

Acceptance of late work for assessment will be at the discretion of the course coordinator and/or the lecturer concerned. If your assessment is likely to be late, please contact the relevant of these people ***before the assessment is due***. Never assume that an extension will be automatically granted – some courses have the policy of no late work being accepted. A commonly exercised policy is to deduct 10% of the total marks for each day that the work is late, where weekends and public holidays also count as such days.

Marks and Grades | Taumata Ako

The following numbers should be considered as a guide to the expected grades under normal circumstances.

Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level; in general this requirement will not be applied at 300 level, but if it is then the course coordinator will inform the class and it will result in a final grade no higher than a C–.

Grade:	**A+**	**A**	**A−**	**B+**	**B**	**B−**	**C+**	**C**	**C-**	**D**	**E**
Minimum mark %:	**90**	**85**	**80**	**75**	**70**	**65**	**60**	**55**	**50**	**40**	**0**

The School reserves the right to adjust this mark/grade conversion, up or down, to achieve consistency of assessments standards.

Reconsideration of Grades

Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Director of Undergraduate Studies, Assoc Prof Greg Russell. Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Student Accessibility Services | Te Whaikaha

Students can speak with someone at Student Accessibility Service, phone: 369 3334 (or ext. 93334), email: sas@canterbury.ac.nz).

Academic Advice

Assoc Prof Greg Russell is the coordinator of undergraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Greg.

Staff-Class Rep Liaison

Assoc Prof Greg Russell is in charge of liaison with students in chemistry courses. Your class will appoint a student representative to the liaison committee at the start of the semester. Please feel free to talk to the Academic Liaison or the student rep about any problems or concerns that you might have.

Greg Russell (greg.russell@canterbury.ac.nz, tel. 369 5129)
Director of Undergraduate Studies
School of Physical and Chemical Sciences
2024