School of Physical and Chemical Science

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

CHEM 336
Supramolecular Chemistry and Molecular Engineering

0.1250 EFTS 15 Points
First Semester 2022

Description
This course runs in semester one. It counts 15 points towards a Bachelor of Science degree. It is preferably it is taken in conjunction with other 300-level chemistry courses.

Molecular engineering is an area of synthetic chemistry that aims to construct complex functional chemicals with tailored properties. The importance of this field was recognised by the award of the 2016 Nobel chemistry prize for scientists working in this area. One major approach to molecular engineering is via supramolecular chemistry; this involves the use of non-covalent interactions (such as coordination chemistry, hydrogen bonding, π-stacking etc) to form well-defined molecular assemblies. These larger well-defined structures can be created with geometrically interesting shapes and electronic properties. In this course, students will develop an understanding of the synthesis of organic and metal-organic compounds suitable for molecular engineering and how these can be assembled into larger ensembles, such as host-guest complexes. The properties and importance of intermolecular interactions and their translation to functions in chemistry as well in bio-, nano- and materials science will also be discussed.

Timetable
Lectures & Workshops: **3** hours of lectures/workshops/tutorials per week. Details to be confirmed on 'My Timetable' and as agreed with the lecturer from time-to-time within that schedule.

Students should note that in the Science Faculty that the average student is responsible for approximately 4.5 hours of additional study for each hour of lecture/workshop contact time at the 300-level.

Course Co-ordinator
Prof. Paul Kruger, School of Physical and Chemical Science
Room 425 Beatrice Tinsley Building, ext: 94367, Email: paul.kruger@canterbury.ac.nz
Email me if you have any queries about the course.

Assessment
In order, with course component indicated (subject to change):
- Assignments **20**%
- Test (Block 1) **30**%
- Final Examination **50**%

Examination and Formal Tests
Test: 1.5 hour, details to be advised.
Exam: 3 hours, details to be advised.

Textbooks
The general textbooks for the course are:

Jonathan W. Steed, Jerry L. Atwood, '*Supramolecular Chemistry*', 2nd Edition; ISBN: 978-1-118-68150-3.

Specific references to book chapters, review articles, research papers, and other books will be made through Learn.

Prerequisites/Restrictions
P: CHEM242 (BCHM206) or CHEM251
Web-based resources: Various learning resources (lecture material, reference links, quizzes, discussion forums etc.) for this course are available via the University of Canterbury's *Learn* web site -- http://learn.canterbury.ac.nz/. This site will also be used regularly as a means of communication and information distribution for all of your Canterbury courses. You should familiarise yourself with *Learn* as soon as possible.

Goal of the Course
This course will serve to introduce important concepts in the field of supramolecular chemistry and molecular engineering. The goals of this course are 1) to familiarize students to the different methods and types of chemical systems used for the assembly of complicated molecular architectures and functional molecules; 2) to help students obtain the essential knowledge needed to critically examine modern scientific research related to supramolecular chemistry and molecular engineering; 3) show how the concepts and tools of supramolecular chemistry are applied in other areas of chemistry and biology; and, 4) be able to critically examine and discuss the properties of supramolecular architectures and engineered products.

Learning Outcomes (see also detailed Learning Objectives after Course Content, below)
- Develop the ability to apply scientific principles and concepts.
- Develop problem-solving and numeracy skills.
- Understand, evaluate, access and critically review new chemical information.
- Demonstrate the ability to think independently about chemical concepts.
- Develop a more in-depth knowledge of chemistry beyond the molecule; the chemistry of intermolecular bonds.
- Know the concepts and phenomena of supramolecular chemistry and understand the role of the weak interactions.
- Communicate effectively in written English and chemical diagrams.

Transferable Skill Register
As a student in this course I will develop the following skills:

- Problem solving. This is a key skill that is transferable to most careers.
- Pattern spotting and logical analysis. A key feature to synthetic chemistry is the ability to understand similarities between processes and use this pattern recognition to address complex issues in a logical fashion.
- Critical analysis of data. This is a key skill that is transferable to most careers
- Three-dimensional spatial awareness. The ability to think about molecules and chemical reactions in three dimensions is highly useful transferable skill.
- Science communication. A particularly important skill is being able to communicate scientific principles.

Summary of the Course Content

BLOCK 1: 18 (12 + 6) Lectures/Problem-solving workshops
SUPRAMOLECULAR AND METALLOSUPRAMOLECULAR CHEMISTRY

Part 1 will introduce supramolecular chemistry (the chemistry of non-covalent interactions), molecular engineering and nanomaterials. Self-assembly processes in organic systems. Catenanes, rotaxanes, pseudo-rotaxanes. Synthetic strategies for their preparation. Main supramolecular forces involved in such assemblies. Examples of each type. Self-assembly processes in metal-containing compounds. Using coordination bonds to prepare large supramolecular assemblies. Cages, macrocycles and catenanes. Polymeric materials and grids. Nano-capsules and containers. Discussion of main synthetic strategies used for their preparation. Potential uses of such assemblies as nano-reactors and for transport (e.g., drug-delivery). Molecular switches and machines. Use of supramolecular forces to assemble components that respond to external stimuli. Functional supramolecular systems and the role of supramolecular chemistry in materials chemistry and biology/medicine.

Part 2 will then introduce the design principles used for the formation of crystalline and polymeric materials constructed using, hydrogen-bonds, metal-ligand coordination, and reversible covalent bonds. Part 2 will build upon fundamental aspects of transition metal coordination chemistry and supramolecular chemistry learned in Part 1. Emphasis will be on understanding the design features, synthetic methodology and potential applications of transition metal coordination polymers (CPs), metal-organic frameworks (MOFs), hydrogen-bonded-organic frameworks (HOFs) and covalent-organic frameworks (COFs). Applications of these materials to areas such as gas storage and separations, catalysis and optics will be discussed. Where possible, topics will be taken from the most recent literature on the subject.

Lecturer: Prof. Paul Kruger, Room 425 Beatrice Tinsley Building, ext. 94367. paul.kruger@*canterbury.ac.nz*

BLOCK 3: 12 (9 + 3) Lectures/Problem-solving workshops
SUPRAMOLECULAR PHOTOCHEMISTRY

Molecular engineering through supramolecular chemistry has as one of its primary goals the creation of functional assemblies. We will discuss how light can be used to drive function and reactivity in molecules, with a specific focus on larger systems. These sessions will provide an introduction into how light interacts with molecules, how the interaction with light can be used to understand supramolecular chemistry, and how light can be used to drive molecular motion.

Lecturer: Dr Chris Fitchett, Beatrice Tinsley 424, ext. 95344. chris.fitchett@*canterbury.ac.nz*

GENERAL INFORMATION 2022

Chemistry Department Policy on 'Dishonest Practice'
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 ('Academic Integrity and Breach of Instruction Regulations').

The Department of Chemistry upholds this policy. It considers plagiarism, collusion, copying, and ghost writing to be unacceptable and dishonest practices:

- ***Plagiarism*** 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.
- ***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) (with, or without payment) to prepare all or part of an item of work submitted for assessment.

Additional Information

Special consideration of assessment*:** If you feel that illness, injury, bereavement or any other critical extenuating circumstance beyond your control has prevented you from completing an item of assessment or affected your performance in that assessment, you may apply for special consideration. Special consideration is not available for items worth less than 10% of the course. Applications for special consideration should be made **within five days** of the due date for the work or examination. In the case of illness or injury, medical consultation should normally have taken place shortly before, or within 24 hours after, the due date for the required work or the date of the test or examination. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. ***You have the right to appeal any decision.

Extensions of deadlines: Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator.

Late withdrawal from the 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*:** 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: these can be found on our website using the link below:
www.chem.canterbury.ac.nz/for/undergraduate.shtml

***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 will be at the discretion of the course coordinator. Please contact the coordinator if your assessment is likely to be late.

Marks and Grades: The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

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

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 (phone 3694228). 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.

Students with Disabilities: Students with disabilities should speak with someone at Equity and Disability Service, phone: 369 3334 (or ext. 93334), email: eds@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
2022