School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

# CHEM 437
# Supramolecular Chemistry

0.125 EFTS 15 Points
First Semester 2022

**Description**
This course is about supramolecular chemistry at a higher level. Supramolecular chemistry is an area of chemistry that aims to construct complex functional chemicals with tailored properties, using non-covalent interactions (such as coordination bonds, hydrogen bonding, π-stacking etc.) to form well-defined molecular assemblies. These larger well-defined structures can be created with geometrically interesting shapes and useful properties. In this course, students will develop an understanding of the synthesis of compounds suitable for supramolecular chemistry and how these can be assembled into larger ensembles, such as host-guest complexes, interlocked molecules, molecular machines, coordination polymers, metal-organic frameworks and covalent organic frameworks. The properties and importance of intermolecular interactions and their translation to functions in chemistry as well in bio-, nano- and materials science. This course will use the example of the photochemistry of supramolecular assemblies to illustrate the usefulness engineered molecular systems. The production of hydrogen through artificial photosynthesis will be discussed in detail.

**Timetable**
***Lectures:*** Two hours of lectures per week. Details to be confirmed on 'My Timetable' and the Web.
***Tutorials:*** One hour of tutorials per week in weeks 2, 4 and 6 of each lecture block. Details to be confirmed on 'My Timetable' and the Web.

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 at 400-level.

**Course Coordinator**
Professor Paul E. Kruger, School of Physical and Chemical Sciences, Room 425 Beatrice Tinsley Building, email: paul.kruger@canterbury.ac.nz

**Assessment**
- Assignments **40**%
- Final Examination **60**%

**Examination and Formal Tests**
***End of year Exam:*** Three hours, with questions from Paul Kruger and Chris Fitchett

**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**
P: CHEM336

**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 your Canterbury courses. You should familiarise yourself with *Learn* as soon as possible.

**Goal of the Course**
This course will serve to expand upon the important concepts in the field of supramolecular chemistry as understood by synthetic chemists. 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; 3) show how the concepts and tools of supramolecular chemistry are applied in other areas of chemistry, biology, medicine, analytical and materials chemistry; and, 4) be able to critically examine and discuss the synthesis and physical properties of supramolecular architectures.

**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**

The topics coved by this course are:

**BLOCK 1: 15 (12 + 3)** Lectures/Problem-solving workshops
***Coordination Polymers: From Crystal Engineering to Metal-organic Framework (MOF) Materials***

This series of lectures will introduce the design principles used for the formation of crystalline and polymeric materials constructed using, hydrogen-bonds, metal-ligand coordination, and reversible covalent bonds. Much of the course material will build upon fundamental aspects of transition metal coordination chemistry and supramolecular chemistry (the chemistry of non-covalent interactions). 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 E. Kruger, email: paul.kruger@canterbury.ac.nz

**BLOCK 2: 15 Sessions (**including Lectures and Problem-solving workshops)
***Title:*** **Photochemistry of Supramolecular Assemblies**

This section of the course will introduce and discuss the Photochemistry of Supramolecular Assemblies. The interaction of light with molecules and supramolecules has been used to drive assembly processes, along with functioning nanomaterials. It is also a core component of the processes of natural and artificial photosynthesis. We will discuss how photochemistry is used to analyse the formation of rotaxanes. We will also discuss energy transfer in detail, and how it can be used to enhance our understanding of molecular assemblies. We will discuss both natural and artificial photosynthesis extensively, and how supramolecular principles can be used to drive these photochemical processes.
**Lecturer:** Dr Chris Fitchett, ext. 95344. *chris.fitchett@canterbury.ac.nz*

## SPECIFIC LEARNING OBJECTIVES

**BLOCK 1:**

At the end of this lecture block you should be able to:

- Understand the chemistry and properties of transition metal coordination polymers (CPs).
- Understand the chemistry and properties of metal-organic frameworks (MOFs).
- Understand the chemistry and properties of hydrogen-bonded-organic frameworks (HOFs).
- Understand the chemistry and properties of and covalent-organic frameworks (COFs).
- Be able to describe why they are important, how they are prepared, and what their potential uses are.
- Achieve a detailed understanding of the design features and preparative methods utilised in the synthesis of CP, MOF, HOF and COF materials and to obtain an in-depth knowledge of the physical and chemical applications of these materials.

**BLOCK 2:**

At the end of this lecture block you should be able to:

- Apply the basic concepts of photophysics and photochemistry to supramolecular assemblies;
- Identify how charge-transfer transitions and the formation of excimers and exciplexes has been used to monitor rotaxane and catenane formation;
- Describe and predict the appearance of absorption, emission and excitation spectra of supramolecular assemblies;
- Describe how energy transfer between molecules, and the requirements of these processes;
- Explain how energy-transfer can be used in the construction of engineered molecular systems;
- Discuss how the photochemical characteristics of the components of natural photosysnthetic systems affect their reactions;
- Critically discuss how the development of water splitting catalysts can be used to show the requirements of the components of an artificial supramolecular photosynthetic system.
- Predict how components will interact in an artificial supramolecular photosynthetic system.

# GENERAL INFORMATION 2022

**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 School of Physical and Chemical Sciences 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.**

***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, and a C- at 300 level.***

| **Grade:** | **A+** | **A** | **A−** | **B+** | **B** | **B−** | **C+** | **C** | **C-** | **D** | **E** |
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| **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 Coordinator of 400-level studies, Dr Sarah Masters (Room 422, Beatrice Tinsley Building, phone 369 4229). 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*****:** Dr Dan Foley is the coordinator of postgraduate 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 postgraduate studies should get in contact with Dan.

Dan Foley
Coordinator of Postgraduate Studies
School of Physical and Chemical Sciences
2022