CHEM 710/7100: Catalysis - Principles and Industrial Applications

Lecturer: Marcel Schlaf MACN 314A, x 53002, mschlaf@uoguelph.ca

Objective of the course: This course will provide an introduction and overview of the field of catalysis using heterogeneous metal/metal oxide and transition metal complexes focusing on

- general principles and reaction patterns of catalytically active transition metal centres and metal/metal oxide surfaces
- mechanisms: kinetic and thermodynamic parameters and how to determine them
- activation of small molecules such as hydrogen, carbon monoxide, carbon dioxide, methane, ethylene, propylene, ethylene oxide, etc.
- large scale industrially relevant processes and their socio-economic importance

The ultimate objective of the course is to provide you with the know-how to understand (or at least make some educated guesses on) the mechanisms of any catalyzed reactions and have some insight into the principles of catalyst, reaction and process design. The course will be - as much as possible - conceptual in nature and thus should be suitable for students in any field of chemistry (inorganic, organic, physical and analytical) with 3rd year level undergraduate courses in inorganic and organic chemistry.

Evaluation

Midterm:	40 %
Presentation	30 %
Research proposal (as take-home final)	30 %

Each student in the course will be required to give a 30-40 min. presentation (PowerPoint or OpenOffice/max. 30 slides) on a topic of his/her choice within the field of catalysis. In order to coordinate this effort and avoid overlap, I will suggest and discuss potential topics in the first class.

The final exam will be take-home in the form of a research proposal in NSERC format (5 pages + 1 page literature) on a specific topic of your choice within the field of homogeneous catalysis. **The proposal and presentation cannot be on the same topic.**

Guidelines on the preparation of NSERC proposals can be found on the NSERC website at www.nserc.ca. The proposal should give a brief 2-2 1/2 pages mini-review of the (patent) literature relevant to your chosen topic and include mechanistic and/or synthetic discussion and a 2 -2 1/2 page description of the actual work to be done outlining the conceptual and experimental approach.

Time: Monday evenings, 19:00 – 21:30 h
Location: Mini-Link room, (C2-278/MACN-203)
Start: 11/09/2017
No class on 09/10/2017 (Thanksgiving)
Midterm (in class): 30/10/2017
Student Lectures: 06-13-20-27/11/2017 (with 8-9 students we will have two presentations/date)
End: 27/11/2017
Due date for take-home exam (research proposal): 01/12/2017
Required mode of submission of your research proposal is as a word processor or pdf file by e-mail to mschlaf@uoguelph.ca or by upload to the Course Cloud (login & password to be announced).

Tentative topics to be covered in lectures:

1. What is catalysis ? Some simple truth and definitions: TOF, TON, catalyst life-times and space-time yields.
2. Homogeneous vs heterogeneous catalysts.
3. Heterogeneous catalysts: types of catalysts, active sites and defects.
4. Synthesis and characterization of metal and metal oxide catalysts.
5. Types of reactors and some important heterogeneously catalyzed processes.
6. Homogeneous catalysts: Overview of types of ligands and their electronic and steric properties. Reaction patterns of transition metal centres and their coordinated ligands.
7. The tools of the trade: mechanistic investigations through thermodynamic, kinetic and isotope labelling studies.
8. Two historical perspectives on homogeneous catalysts: The Wacker process and Wilkinson's Catalyst.
9. Hydrogenation and hydrogenolysis reactions beyond Wilkinson: The Shvo and Noyori systems: ionic and enantioselective hydrogenations.
10. Oxidation and epoxidation beyond Wacker: The search for efficient and "green" aerobic oxidation catalysts. The Sharpless catalyst.
11. Adding carbons I: Hydroformylation, hydrocyanation, carbonylation, Fischer-Tropsch chemistry and related reactions - the Monsanto process.
12. Adding carbons II: Oligomerization and dimerization reactions. The Shell Higher Olefin Process (SHOP). Metallocenes and other single-site polymerization catalysts. Metathesis reactions and ROMP using Grubb's catalyst.
13. The Holy Grail I: Catalytic C-H bond activation in simple hydrocarbons: The Catalytica process (Periana Catalyst) and related fundamental processes.
14. The Holy Grail II: Catalytic Hydrodeoxygenation of biomass to fuel and chemicals.
15. Cross-coupling and other miscellaneous reactions: Heck, Stille, Sonogashira, Hartwig, Buchwald, etc.

Required University of Guelph and University of Waterloo Statements for Course Outlines

For University of Waterloo Students

Academic Integrity: In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect and responsibility. [Check www.uwaterloo.ca/academicintegrity/ for more information.]

Appeals: A decision made or penalty imposed under Policy 70 (Student Petitions and Grievances) (other than a petition) or Policy 71 (Student Discipline) may be appealed if there is a ground. A student who believes he/she has a ground for an appeal should refer to Policy 72 (Student Appeals) www.adm.uwaterloo.ca/infosec/Policies/policy72.htm .

Discipline: A student is expected to know what constitutes academic integrity [check www.uwaterloo.ca/academicintegrity/ to avoid committing an academic offence, and to take responsibility for his/her actions. A student who is unsure whether an action constitutes an offence, or who needs help in learning how to avoid offences (e.g., plagiarism, cheating) or about "rules" for group work/collaboration should seek guidance from the course instructor, academic advisor, or the undergraduate Associate Dean. For information on categories of offences and types of penalties, students should refer to Policy 71, Student Discipline, www.adm.uwaterloo.ca/infosec/Policies/policy71.htm. For typical penalties check Guidelines for the Assessment of Penalties, www.adm.uwaterloo.ca/infosec/guidelines/penaltyguidelines.htm

Grievance: A student who believes that a decision affecting some aspect of his/her university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy 70, Student Petitions and Grievances, Section 4, www.adm.uwaterloo.ca/infosec/Policies/policy70.htm. When in doubt please be certain to contact the department's administrative assistant who will provide further assistance.

Note for Students with Disabilities: The Office for persons with Disabilities (OPD), located in Needles Hall, Room 1132, collaborates with all academic departments to arrange appropriate accommodations for students with disabilities without compromising the academic integrity of the curriculum. If you require academic accommodations to lessen the impact of your disability, please register with the OPD at the beginning of each academic term.

Turnitin.com: Plagiarism detection software (Turnitin) will be used to screen assignments in this course. This is being done to verify that use of all material and sources in assignments is documented. In the first week of the term, details will be provided about the arrangements for the use of Turnitin in this course.

Note: students must be given a reasonable option if they do not want to have their assignment screened by Turnitin. See: http://uwaterloo.ca/academicintegrity/Turnitin/index.html for more information.

For University of Guelph Graduate Students

The following are standard statements for inclusion in all course outlines. Some departments or colleges may also elect to post this information on a common website and link to such sites in the course outline. However, it is strongly recommended that statements on academic misconduct and links to the academic misconduct section of the academic calendars be included in all course outlines.

E-mail Communication: All students are required to check their University of Guelph e-mail account regularly. E-mail is the official route of communication between the University and its students.

When You Cannot Meet a Course Requirement: When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course in writing, with your name, id#, and e-mail contact. See the graduate calendar for information on regulations and procedures for Academic Consideration.

Drop Date: The last date to drop one-semester courses, without academic penalty, is Friday 31 October 2014. Two-semester courses must be dropped by the last day of the add period in the second semester. Refer to the Graduate Calendar for the Schedule of Dates.

Academic Misconduct: The University of Guelph is committed to upholding the highest standards of academic integrity and it is the responsibility of all members of the University community – faculty, staff, and students – to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection. The Academic Misconduct Policy is detailed in the Graduate Calendar.

Recording of Materials: Presentations which are made in relation to course work—including lectures—cannot be recorded in any electronic media without the permission of the presenter, whether the instructor, a classmate or guest lecturer.

Resources: The Graduate Calendar is the source of information about the University of Guelph's procedures, policies and regulations that apply to graduate programs:
http://www.uoguelph.ca/registrar/calendars/graduate/current/