CHEM*7100/710
Supramolecular and Nanostructured Materials

Winter 2013 – Course Outline

The main objective of this course is to show how the concepts of supramolecular chemistry and nanoscience are utilized in the design of new materials. The course provides a short overview of all main aspects of self-assembled nanostructured objects, from the smallest host-guest complexes to sophisticated molecular devices and infinite multicomponent systems. **Credits**: 0.5.

Website http://www.chemistry.uoguelph.ca/soldatov/C7100

Schedule Jan 8th – Apr 2nd (first class is Jan 8th; no class on Feb 19th); exam on Apr 9th
Tuesdays, 7:00 pm – 9:30 pm
Main Link Room (Guelph: MACN-101; Waterloo: EIT-2053)

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Evaluation Assignment I (due on Feb 12th, 25%); Assignment II (Mar 19th; 25%), in-class presentation on a topic relevant to the student's research (Apr 2nd; 25%); final exam (Apr 9th; 25%)

Contents

1 *Introduction*: Supramolecular chemistry, nanoscience and materials. The size-property relationship (single molecule – nano-sized object – bulk material). Compounds, mixtures, phases and materials. Supramolecular, nanostructured and hybrid materials.

2 *Oligomolecular associates*. Molecular clathrates. Self-assembling capsules and rosettes. Rotaxanes, catenanes and knots. Helicates. *Macrocyclic receptors*: crown-ethers, cyclodextrins, calixarenes and others. Template effect. Complementarity and preorganization.

3 *Polymolecular self-assembly*. Viruses. Nanotechnology vs nanochemistry. Nanoparticles. Infinite nanoobjects. Nanostructured materials.

4 *Non-covalent interactions*. Weak vs labile interactions. Coordination bonds. Hydrogen bonds. Etter's rules. Supramolecular synthon. Molecular tectonics. Van der Waals interactions. Molecular crystals. Packing efficiency and energy of the molecular crystal framework. Design of new host geometries.

5 *Crystal engineering and solid state organic synthesis*. Crystals and photochemistry. Confined spaces in solids as nanoreactors. Coordination polymers. Porous metal-organic frameworks.

6 *Physicochemical basis* for the formation of supramolecular phases driven by thermodynamics. Sorption, clathration, encapsulation and other types of inclusion behavior. The formation of clathrates. Pharmaceutical co-crystals. Blue reaction of iodine. *Experimental methods*: overview.

7 *Inclusion compounds*: overview. Hydroquinone and analogs. Gas hydrates. Metal complexes as hosts. Tubulates based on urea and other organics. Cholic and other bile acids. Peptide nanotubes and layered structures. Graphite intercalates. Clays.

8 *Zeolites*: structure, properties, synthesis, applications. *Mesoporous silicas* and related solids. Organic zeolite mimics. Imprinted polymers.

9 *Non-solid or non-crystalline soft materials*. Dendrimers. Liquid crystals. Liquid clathrates. Gels. Fibrils and fibers.

10 *Molecular devices*. Biotransport. Supramolecular catalysis and artificial enzymes. Other examples of biomimics. Molecular machines.

Resources Lecture Notes will be posted on the course website in advance of the classes
A number of general texts and web resources are available and may be used; some texts are listed below:

JW Steed, DR Turner, KJ Wallace, *Core Concepts in Supramolecular Chemistry and Nanochemistry*, Wiley, 2007

JW Steed, JL Atwood, *Supramolecular Chemistry*, Wiley, 2000

JL Atwood, JED Davies, DD MacNicol, F Vögtle (eds.), *Comprehensive Supramolecular Chemistry*, Elsevier, 1996, volumes 1-11.

General policies and regulations:

E-mail Communication: As per university regulations, all students are required to check their university 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 instructor in writing, with your name, id#, and e-mail contact. Follow the following links for regulations and procedures for Academic Consideration:
http://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/
http://www.registrar.uwaterloo.ca/students/accom_illness.html

Drop Date: The last date to drop the course, without academic penalty, is 8 March 2012.

Copies of out-of-class assignments: Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

Accessibility: Providing services for students is a shared responsibility among students, faculty and administrators. This relationship is based on respect of individual rights, the dignity of the individual and the university community's shared commitment to an open and supportive learning environment. Students requiring service or accommodation, whether due to an identified, ongoing disability or a short-term disability should contact the Centre for Students with Disabilities as soon as possible. For more information see the following websites:
http://www.uoguelph.ca/csd/
http://www.studentservices.uwaterloo.ca/disabilities/

Academic Misconduct: The 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.
Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor. For further details see:
http://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/
http://www.adm.uwaterloo.ca/infosec/Policies/policy71.htm

Recording of Materials: Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

Resources: The Academic Calendars are the source of information about the university procedures, policies and regulations which apply to undergraduate, graduate and diploma programs:
http://www.uoguelph.ca/registrar/calendars/index.cfm?graduate
http://gradcalendar.uwaterloo.ca/group/Gen-Info-Regs