New York University
Department of Chemistry

CHEM-GA 1315 Supramolecular Chemistry
Spring 2017

Instructor Prof. Daniela Buccella, dbuccella@nyu.edu
Silver 827, Biomedical Chemistry Institute

Lectures Tuesdays and Thursdays 8:00 am – 9:30 am
Waverly Room 569

Office hours By appointment, Silver 827

Course Summary
Described by J. M. Lehn as the "chemistry beyond the molecule", supramolecular chemistry is an interdisciplinary field that covers the physical, chemical and biological properties of complex chemical species held together mainly by non-covalent interactions. This graduate-level course provides an introduction to the field, using examples from the recent literature as a starting point to examine the intermolecular forces that dictate the formation of supermolecules and supramolecular assemblies and their properties. Discussion topics include basics of molecular recognition, folding, self-assembly, supramolecular reactivity and function. Physical methods employed to study supramolecular systems are introduced throughout the course.

Pre-requisites
Physical Organic Chemistry or strong background in organic chemistry recommended. Undergraduate students must receive approval from the instructor to enroll in this course.

Principal reading material (recommended, not required)
- Anslyn & Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2006. ISBN: 978-1891389313
- Connors, *Binding Constants,* John Wiley & Sons, 1987.
- Martell & Hancock*, Metal Complexes in Aqueous Solutions*, Plenum Press, 1996.
- Israelachvili, *Intermolecular and Surface Forces, 3rd Ed.* Elsevier, 2011. ISBN: 978-0-12-375182-9
- Lehn, *Supramolecular Chemistry,* VCH, 1995
- Steed & Atwood*, Supramolecular Chemistry,* John Wiley & Sons, 2000.

Other reading resources, including articles of the primary literature, will be assigned in class to cover specific topics.

Topics outline
1. Introductory concepts
- Terminology and definitions in supramolecular chemistry.

2. Solutions and intermolecular forces
- Solvent and solution properties.
- Intermolecular forces: Ion pairing, ion-dipole and dipole-dipole interactions; hydrogen bonding; pi interactions.

- Binding: binding constants, physical methods for binding constant determination.

3. Interactions in the solid state

4. Molecular recognition
- Complementarity and preorganization.
- Shapes and homochirality.
- Molecular recognition in water; the hydrophobic effect.
- Coordination chemistry and the chelate effect.
- Cooperativity and multivalency.

5. Folding of biological and synthetic polymers

6. Self assembly

7. Function
- Supramolecular reactivity and catalysis.
- Responsive materials.
- Molecular machines.

Assignments and grading

The grade for the course will be determined based on problem sets and in-class examinations according to the following scheme:

Exam 1	30%	03/07/17
Exam 2	30%	05/04/17
In-class presentation	15%	(topic to be approved by the instructor at least two weeks in advance)
Problem sets/Quizzes	25%	

Exams:

In-class exams will be 75 min in duration; students arriving late will not be given extra time. The use of notes, handouts, and/or other materials during the exam is not permitted, unless indicated by the instructor in advance. Students must work individually. Make-up exams will not be allowed with the exception of documented cases of illness. The content of exams is cumulative.

Presentations:

In-class presentations should be 20 min (17 min presentation + 3 min for questions) on literature examples covering a topic in supramolecular chemistry. The topic must be approved by the instructor at least two weeks in advance of the presentation date.

Problem sets:

Answers to problem sets must be handed in at the beginning of class on the corresponding due date. No credit will be given for problem sets received late. Students are allowed to discuss with each other the content of the problem sets. Answers sets, however, must be crafted individually and must reflect each student's independent reasoning for the solution of each problem. Neither joint work nor copies of other student's answers will be accepted. Students should review NYU's policy on academic integrity at: http://www.nyu.edu/about/policies-guidelines-compliance/policies-and-guidelines/academic-integrity-for-students-at-nyu.html.

Quizzes:

Short quizzes will be given periodically in class (unannounced).