CHEM-GA 1315  Supramolecular Chemistry - Fall 2019

Instructor Information
Prof. Daniela Buccella,
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Office: Silver 827, Biomedical Chemistry Institute
Office hours: by appointment

Course Information
Mondays and Wednesdays, 12:30 – 1:45 pm
7 East 12th St, Room LL31

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)
- Martell & Hancock, Metal Complexes in Aqueous Solutions, Plenum Press, 1996.
- Lehn, Supramolecular Chemistry, VCH, 1995

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; halogen bond; pi interactions.
   - Binding: binding constants, physical methods for binding constant determination.

3. **Molecular recognition**
   - Complementarity and preorganization.
   - Molecular recognition in water; the hydrophobic effect.
   - Coordination chemistry and the chelate effect.
   - Cooperativity and multivalency.

4. **Folding of biological and synthetic polymers**

5. **Self assembly**

6. **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:

<table>
<thead>
<tr>
<th>Assignment</th>
<th>Weight</th>
<th>Due Date</th>
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</thead>
<tbody>
<tr>
<td>Exam 1</td>
<td>30%</td>
<td>10/23/19</td>
</tr>
<tr>
<td>Exam 2</td>
<td>30%</td>
<td>12/11/19</td>
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<tr>
<td>Quizzes</td>
<td>15%</td>
<td>Announced in class</td>
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<tr>
<td>In-class presentation</td>
<td>10%</td>
<td>TBD. (Topic to be approved by the instructor at least two weeks in advance)</td>
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<tr>
<td>Problem sets</td>
<td>15%</td>
<td>Announced in class</td>
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**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 exams 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.

**Quizzes:**
Short quizzes (15 min) will be given periodically in class.

**Presentations:**
In-class presentations should be based on literature examples covering recent topics in supramolecular chemistry. Topics should illustrate and expand upon concepts discussed in class, and 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/thought process toward 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.