School of Interdisciplinary Engineering and Sciences (SINES)
National University of Sciences & Technology (NUST)

Title : Concepts in Supramolecular Chemistry
Code : CSE-917
Pre-requisite: Basic Knowledge of Chemistry
Credit Hours: 3-0

Description: This course draws together concepts in inorganic, organic and some physical chemistry to study the behavior and applications of supramolecular assemblies. Supramolecular Chemistry describes the chemistry of the interaction between discrete molecules and the collective properties of this interaction.

Objectives:

Main Objectives of the program under which course will be designed are,

a) To introduce students to the basic concepts of host-guest (supramolecular) chemistry and molecular recognition.
b) To build fundamental knowledge in organic and inorganic chemistry to illustrate the relationship between these topics and supramolecular chemistry.
c) To use relevant chemical concepts to analyze aspects of supramolecular chemistry and their applications using current examples.

Outcomes: Students will explore the principles of molecular recognition, including host-guest interactions and the concept of supramolecular self-assembly. They will study the factors influencing molecular recognition and the design principles for creating specific host-guest complexes.

Course Contents:

1. Concepts
2. Definition and Development of Supramolecular Chemistry
3. Classification of Supramolecular Host–Guest Compounds
4. Receptors, Coordination and the Lock and Key Analogy
5. Binding Constants
6. Thermodynamic and Kinetic Selectivity and Discrimination
7. Nature of Supramolecular Interactions
8. Solvation and Hydrophobic Effects
9. Supramolecular Concepts and Design
10. The Supramolecular Chemistry of Life
11. Biological Inspiration for Supramolecular Chemistry
12. DNA & Enzyme Binding

Contents with proposed contact hours

Week	Topics
1	Introduction-meaning of Supramolecular Chemistry, phenomenon of molecular recognition and their quantification
2	Building blocks of supramolecular
3	Nature of Supramolecular Interactions

4	Effects of Supramolecular Interactions
5	Binding Constants
6	Types of Supramplecular Host and guests
7	Amphiphilic molecules and their aggregation
8	Kinetics of Host/ guest interactions
9	**Midterm**
10	Supramolecular chemistry on Solids Surfaces
11	Layered surfaces
12	Computational methods and approaches being implemented for deep learning of supramolecular systems
13	Lab: (i) Identification of Host as clatherate or cavitate, (ii) Modeling of non-covalent interactions through MM and QM approaches
14	Catalysis and other applications
15	Semiochemisty-introduction and its role in supramolecular design systems
16	Sensors and information processing
17	Applications in Nanochemistry
18	**ESE**

Text Books/Reference Material:

1. Steed J. W., Atwood J. L.: Supramolecular chemistry. John Wiley & Sons Ltd, Chichester 2000. (CS)
2. Ariga K., Kunitake T.: Supramolecular chemistry: fundamentals and applications: advanced textbook. Springer, Berlin 2005. (CS)
3. Schalley, C.: Analytical Methods in Supramolecular Chemistry. Wiley-VCH Verlag 2007 (CS)
4. Chneider, H.J.: Application of supramolecular chemistry, CRC Press 2012. (CS)
5. Relevant Review, Research articles and Tutorials.

Nature of Assessments:

Homework/ Assignments: 10%
Quizzes: 10%
MSE: 30%
Final Exam: 50%

Comparative Chart:

No	**Topics**	**Proposed**
1.	Introduction-meaning of Supramolecular Chemistry, phenomenon of molecular recognition and their quantification	Retained
2.	Building blocks of supramolecular	Retained
3.	Nature of Supramolecular Interactions	Retained
4.	Effects of Supramolecular Interactions	Retained
5.	Binding Constants	Retained
6.	Types of Supramplecular Host and guests	Retained
7.	Amphiphilic molecules and their aggregation	Retained
8.	Kinetics of Host/ guest interactions	Retained
9.	Supramolecular chemistry on Solids Surfaces	Retained
10	Layered surfaces	Retained
11	Computational methods and approaches being implemented for deep learning of supramolecular systems	Retained
12	Lab: (i) Identification of Host as clatherate or cavitate, (ii) Modeling of non-covalent interactions through MM and QM approaches	Retained
13	Catalysis and other applications	Retained
14	Semiochemisty-introduction and its role in supramolecular design systems	Addition of New Content
15	Sensors and information processing	Addition of New Content
16	Applications in Nanochemistry	Addition of New Content