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

Title : Modeling Polymeric Materials
Code : CSE-918
Pre-requisite: Basic Knowledge of Chemistry
Credit Hours: 3-0

Description: One of basic concepts in the computational simulation progresses is the modeling of polymeric systems. Quantum mechanical calculations from first principles are too exhaustive in this case, as length scales of structural properties as well as time scales of dynamic properties are spread over several orders of magnitude. Thus, mesoscale simulation techniques (combining several atoms or monomers to segments and using more simple potentials) are used as well as force field based atomistic classical dynamics for smaller systems.

Objectives: The objective of this course is to develop computational methods to enable design of polymeric biomaterials with specified bioresponse characteristics. It will also accelerate the discovery of polymeric biomaterials with the goal of bringing regenerative therapies and advanced drug delivery systems. Another important objective will be identifying new synthetic methods to increase the number and chemical diversity and exploration of candidate polymers. Developing computational models for the discovery of new polymeric biomaterials, and computational tools to predict the success of biomaterials in specific medical applications.

Outcomes: The course will equip students with the knowledge and skills to develop mathematical models for predicting the behavior of polymeric materials. Students will learn how to use computational tools and software specifically designed for modeling polymeric materials.

Course Contents:

1. Going From Small Molecules to Large Ones
2. Basic concepts in polymer chemistry.
3. Polymerization reactions-mechanisms
4. Kinetics of polymerization reactions
5. Thermodynamics of polymer systems.
6. Industrially Important Polymers
7. Overview of the Literature
8. The Scope of Quantum Mechanical Calculations for Polymers
9. Modeling polymers;
10. Quantum mechanical calculations;
11. Molecular dynamics methods;
12. Monte Carlo methods
13. Molecular Mechanics and Atomistic Simulations
14. General Principles of Molecular Dynamics
15. General Principles of the Monte Carlo Method
16. Not All Macromolecules are Alike: What Works for Proteins May Not Work for Synthetic Polymers
17. Single Chain Studies

18. Modeling Amorphous Polymers in the Bulk

Contents with proposed contact hours:

Week	Topics
1	Going From Small Molecules to Large Ones
2	Basic concepts in polymer chemistry.
3	Polymerization reactions-mechanisms
4	Kinetics of polymerization reactions
5	Thermodynamics of polymer systems.
6	Industrially Important Polymers
7	Overview of the Literature
8	The Scope of Quantum Mechanical Calculations for Polymers Modeling polymers;
9	**Midterm**
10	Quantum mechanical calculations;
11	Molecular dynamics methods;
12	Monte Carlo methods
13	Molecular Mechanics and Atomistic Simulations
14	General Principles of Molecular Dynamics
15	General Principles of the Monte Carlo Method
16	Not All Macromolecules are Alike: What Works for Proteins May Not Work for Synthetic Polymers, Single Chain Studies
17	Modeling Amorphous Polymers in the Bulk
18	**ESE**

Text Books/Reference Material:

1. Polymer Nanocomposites: Processing, Characterization, and Applications, 2nd Edition (2019) 2nd Edition. JH
2. by Joseph Koo (Author)
3. Computational Modeling of Polymer Composites, 1st Edition (2014), Samit Roy, J.N. Reddy. Taylor and Francis Group.
4. Introduction to Polymers, Third Edition by Robert J. Young. June 27, 2011 CRC Group, Taylor and Francis Group.

Nature of Assessments:

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