PCH235 MOLECULAR MODELING AND SIMULATION

L	T	P	Cr
3	1	0	3.5

Course Objective:

To learn to mimic the real system and phenomena in virtual world using molecular level information and computational resources and to develop and design the novel performance chemicals and materials.

Introduction: Need of molecular modelling and simulation, Postulates of statistical mechanics, Ergodic hypothesis.

Statistical Ensembles and Partition Functions: System and particle partition function and relation to thermodynamics, Micro-canonical ensemble, Canonical ensemble, Isothermal-isobaric ensemble, Grand-canonical ensemble, Gibbs ensemble, Thermodynamic equivalence of ensembles, Ensemble average and time average equivalence.

Empirical Force Field Models: General features of molecular mechanics force fields, Bond stretching, Bond bending, Dihedrals and torsion, Non-bonded interactions, Hard and soft interactions, Electrostatic interactions, Combination/mixing rules, Standard force fields.

Simulation of Ensembles Using Monte Carlo and Molecular Dynamics Methods: Introduction to Monte-Carlo simulation, Importance sampling and the metropolis algorithm, Implementation of metropolis Monte Carlo algorithm, Simulation cell and periodic boundary conditions, Moves and acceptance criteria, Simulations in different ensembles, Multi-canonical Monte Carlo and the transition matrix, Configurational bias Monte Carlo, Calculation of thermodynamic properties, Introduction to molecular dynamics simulation, Initialization and force calculation, Algorithms to integrate the equations of motion, Thermostats and barostats, Autocorrelation functions, Free energy calculations, Molecular dynamics packages, Design and development of novel performance chemicals and materials for applications in polymers, catalysts, pharmaceuticals and solvents.

Course learning outcomes (CLOs):

The students will be able to

1. apply the principles of molecular mechanics in molecular modeling
2. apply various simulation techniques for model solutions
3. use molecular modeling software
4. design and develop novel performance chemicals and materials for applications in polymers, catalysts, pharmaceuticals

Recommended Books:

1. *McQuarrie, D.A.,Statistical Mechanics, University Science Books (2000).*
2. *Frenkel, D.,andSmit, B.,Understanding Molecular Simulation: From Algorithms to*
3. *Applications, Academic Press, (2002).*
4. *Leach, A.R., Molecular Modeling: Principles and Applications, Pearson Education Ltd. (2001).*

Evaluation Scheme:

S.No.	Evaluation Elements	Weightage (%)
1.	MST	30
2.	EST	45
3.	Sessional (may include Assignments/Projects/Tutorials/Quizes/Lab Evaluations)	25