



INTRODUCTION TO MOLECULAR THERMODYNAMICS

PROF. SRABANI TARAPHDER

Department of Chemistry
IIT Kharagpur

TYPE OF COURSE : Rerun | Core | UG

COURSE DURATION : 8 Weeks (21 Feb' 22 - 15 Apr' 22)

EXAM DATE : 23 Apr 2022

PRE-REQUISITES : Introduction to (1) quantum mechanics (2) probability and statistics

INTENDED AUDIENCE : B.Sc. in Chemistry

INDUSTRIES APPLICABLE TO : Chemical and pharmaceutical industries, Software development for molecular modeling

COURSE OUTLINE :

This course is designed to use fundamental concepts of statistical mechanics in simple real world problems. Starting from simple molecular models of systems like solids, liquids and gases, the students would learn how to obtain their thermodynamic properties that are usually measured in experiments.

ABOUT INSTRUCTOR :

Prof. Srabani Taraphder is a theoretical chemist. Her research interest is focused on the physics of biochemical reactions. She uses principles of quantum and statistical mechanics to carry out computer simulation studies of chemical reactions catalyzed by enzymes.

COURSE PLAN :

Week 1: Review of mathematical methods and classical thermodynamics

Week 2: Introduction to micro- and macroscopic states, ensembles

Week 3: Microcanonical ensemble and application to simple non-interacting systems

Week 4: Canonical ensemble and application to simple non-interacting systems

Week 5: Monatomic and diatomic ideal gases

Week 6: Heat capacity of solids – Einstein and Debye model

Week 7: Introduction to classical statistical mechanics and application to real gases and liquids

Week 8: Molecular thermodynamics of simple chemical reactions and transition state theory