Introduction to Molecular Thermodynamics

Chemistry and Biochemistry

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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.

Pre Requisites: : Introduction to (1) quantum mechanics (2) probability and statistics
Core/Elective: : Core
UG/PG: : UG
Industry Support : Chemical and pharmaceutical industries, Software development for molecular modeling

Course Intro: : 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.

COURSE PLAN

SL.NO	Week	Module Name
1	1	Review of mathematical methods and classical thermodynamics
2	2	Introduction to micro- and macroscopic states, ensembles
3	3	Microcanonical ensemble and application to simple non-interacting systems
4	4	Canonical ensemble and application to simple non-interacting systems
5	5	Monatomic and diatomic ideal gases
6	6	Heat capacity of solids â€“ Einstein and Debye model
7	7	Introduction to classical statistical mechanics and application to real gases and liquids
8	8	Molecular thermodynamics of simple chemical reactions and transition state theory