



# BASIC THERMODYNAMICS : CLASSICAL AND STATISTICAL APPROACHES

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**PRE-REQUISITES :** It requires 12th standard mathematics. It requires the knowledge of calculus(differentiation) and basic probability.

**INTENDED AUDIENCE :** First-year undergraduates of B.Sc. in Chemistry. Some of the concepts are helpful for M.Sc. students in physical chemistry and doctoral students who would need to refresh their concepts of thermodynamics.

**INDUSTRIES APPLICABLE TO :** This course will be helpful for all students across disciplines because of its fundamental nature.

### COURSE OUTLINE :

In this course, we will now find out the reason for changes in matters (Chemical Principles II). The earlier course, Chemical Principles I, deals with the matter itself, and the understanding of it comes from quantum mechanics. However, for the change of matter, thermodynamics says the final word. The most critical quantity in thermodynamics is the entropy, and this course is all about understanding entropy and related thermodynamic potentials. Although classical thermodynamics was developed from observations and heuristic understanding, statistical thermodynamics provides a microscopic basis of it. In this course, a holistic approach covering three different approaches (classical, statistical, and postulate-based) of thermodynamics will be covered. The objective of this course is demystification the enigma of entropy.

### ABOUT INSTRUCTOR :

Arnab Mukherjee did his B. Sc from Jadavpur University, Kolkata in 1998. He then joined Indian Institute of Science, Bangalore as an integrated Ph.D. student in chemical sciences. He completed his Ph.D. from S. S. C. U. department of IISc Bangalore in 2005 under the supervision of Professor Biman Bagchi. Dr. Mukherjee then went for his postdoctoral research to Ecole Normale Supérieure, Paris, France from 2005 to 2007 and then to the University of Colorado, Boulder from 2007 to 2009. He then joined IISER Pune as an assistant professor in November 2009. He became an associate professor in 2015. Dr. Mukherjee works on the computational biophysics area such as drug-DNA intercalation, DNA structural changes, single water entropy, protein folding, protein-DNA interaction, dynamical recrossing, internal friction in proteins, etc. He also collaborates with experimental colleagues in various projects such as synthetic ion channels, spectroscopic investigation of molecular recognition, etc. He has over eight years of teaching experience at IISER Pune.

### COURSE PLAN :

**Week 1:** Thermodynamics everywhere; historical development of thermodynamics; Zeroth Law of Thermodynamics and concept of temperature;

**Week 2:** Discussion on internal energy heat and work; First Law of Thermodynamics

**Week 3:** State function and path function; calculation of p-V work

**Week 4:** Heat capacities; Joule & Joule-Thomson expansion; Some practice problems; thermochemistry

**Week 5:** Second Law of thermodynamics (various statements and their equivalence); Carnot cycle; definition of entropy

**Week 6:** Heat engines and their efficiencies; practice problems on the classical second law

**Week 7:** Statistical Formulation of the Second Law (probability overview; Boltzmann formula, distribution of energy)

**Week 8:** Statistical formulation of the Second Law continued (the most probable distribution, Boltzmann distribution)

**Week 9:** Calculation of entropy for various processes using Boltzmann entropy formula

**Week 10:** Fundamental equation and entropy postulates; introduction to free energies

**Week 11:** Maxwell Relations and conversion of thermodynamic derivatives

**Week 12:** Applications of free energy