



# THERMODYNAMICS: CLASSICAL TO STATISTICAL

## PROF. SANDIP PAUL

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Biochemistry IIT Guwahati

**INTENDED AUDIENCE:** Any interested learners

### COURSE OUTLINE :

This course is intended for final year BSc (in Chemistry) as well as for MSc (in Chemistry) and PhD (in Chemistry) students and it is assumed that no previous knowledge of the subject is required. Moreover, this course demonstrates the form physical and statistical basis of thermodynamics by showing how the properties of macroscopic systems are direct consequences of the behaviors of their elementary constituents. Thus this course will give the students a broader spectrum of skills as well as a better understanding of the physical bases.

### ABOUT INSTRUCTOR :

Prof. Sandip Paul, The broad area of instructor's teaching and research interest is statistical mechanics and its applications to chemistry and biology. Prof. Paul completed his PhD in computational chemistry from Indian Institute of Technology, Kanpur. Later he worked with Prof. Gern Patey of University of British Columbia, Vancouver, Canada and with Prof. Max Berkowitz of University of North Carolina, Chapel Hill, USA for his postdoctoral research. Soon after, he joined in the Department of Chemistry, Indian Institute of Technology, Guwahati as a faculty member. Understanding the effect of osmolytes on the protein conformation, the use of hydrotrope molecules to enhance the aqueous solubility of sparingly soluble drug molecules etc. is the main interest of his research group. He has published 64 journal papers as of now.

### COURSE PLAN :

**Week 1:** Properties of ideal gases and how they differ from real gases, first law of thermodynamics

**Week 2:** Concepts of state and path functions (with examples); Proof of work and heat as path functions and internal energy as state function

**Week 3:** Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solutions; determination of activity, activity coefficients and ionic strength.

**Week 4:** Phase diagram of two component systems (with examples).

**Week 5:** One dimensional random walk and its importance

**Week 6:** Canonical ensemble and calculation of different thermodynamical quantities such as average pressure, average energy.

**Week 7:** Translational partition function

**Week 8:** Rotational and vibrational partition function

**Week 9:** Quantum Statistics of ideal gases. Identical particles and symmetry requirements.

**Week 10:** Quantum distribution functions: Bose-Einstein Statistics

**Week 11:** Ideal Bose gas

**Week 12:** Ortho and para hydrogen