

# ChE665A: Statistical Mechanics and Kinetics for Engineers (3-0-0-9)

**Lecturer:** Professor Vishal Agarwal  
**Office:** 107, Northern Lab II  
**Email:** vagarwal@iitk.ac.in

**Lectures:** Links to the lectures will be sent to you through email.  
**Discussion Hours:** Wednesday, 9:00am to 10:00am  
**Office Hours:** by appointment

**Assessment:** 40% for quizzes, 20% for Project, 40% for end-sem (take-home). 90% attendance is compulsory in the discussion session. **Zero-tolerance policy on academic dishonesty.**

**Assignments:** Reading assignments, and Home assignments (every two weeks).  
 After the due date you will be given one-hour quiz to solve a modified problem picked by me from the assignments (may be open book) or you will be quizzed on the fundamentals taught in the class.

**Examination:** Five quizzes (online for ~ 1hr, best of four will be considered for grading).  
 End-sem (take-home).

**Requirements:** Laptop and high-speed internet.

## Lecture-wise Breakup:

Topics	Lectures <sup>a</sup>
<b>Fundamentals of Equilibrium Thermodynamics:</b> Microscopic and Macroscopic variables, System and Environment in equilibrium, Extensive and Intensive variables, Laws of Thermodynamics, Applications of the second law of thermodynamics, Mathematics of Extensive and Intensive functions.	5
<b>Thermodynamic Stability:</b> Stability criteria and conjugate variables, Application to heat capacities, Applications to phase equilibria, Auxiliary functions, Jacobian method, and Maxwells relations.	5
<b>Foundations of Statistical Mechanics:</b> Ergodic Hypothesis, Spatial and Ensemble averages, Micro- Canonical Ensemble, Canonical ensemble, Quantum and Classical averages, Generalized Ensembles as Legendre transforms, Fluctuations.	6
<b>Statistical Mechanics of Non-Interacting (Ideal) Systems:</b> Statistics of Ideal Systems, Bosons and Fermions, Vibrations in solids as phonon gas, Ideal gas of atoms and molecules, Chemical equilibria in gasses.	8
<b>Non-Ideal Systems (Liquids):</b> Off-Lattice and On-Lattice Models, Virial Theorem, Thermodynamic properties from radial distribution functions, Solvation and Chemical equilibria in liquids.	6
<b>Statistical Mechanics of Non-equilibrium Systems (Dynamics and Relaxation):</b> Phase space, System close to equilibrium, Regression Hypothesis, Time-correlation functions, Fluctuation-Dissipation theorem, Response functions, Chemical Kinetics and Transition state theory, Ficks Law and Self-diffusion, Langevin Equation and Friction	8
<b>Simulations Methods:</b> Molecular dynamics, Monte Carlo, Rare-Event Simulations, Examples and Applications.	2
<b>Total</b>	<b>40</b>

<sup>a</sup>Each lecture is of 50 mins duration

**Teaching Assistants:** Dadi Gowtam (gkchem@iitk.ac.in)  
Soumyadeb Ghosh (soumi@iitk.ac.in)

### References:

- **Text Books on Statistical Mechanics**

- “*Introduction to Modern Statistical Mechanics*”, David Chandler, Oxford University Press, Sep 1987. ISBN-10: 0195042778, ISBN-13: 9780195042771.
- “*Statistical Mechanics*”, Donald A. McQuarrie, University Science Books, June 2000, 2nd Edition, ISBN-13: 978-1-891389-15-3.

- **Other References**

- “*The Principles of Chemical Equilibrium: With Applications in Chemistry and Chemical Engineering*”, by Kenneth Denbigh, Cambridge University Press, March 1981, 4th Edition, ISBN-13: 978-0521281508, ISBN-10: 0521281504.
- “*An Introduction to Statistical Thermodynamics*”, by Terrell L. Hill, Dover Publications, January 1986, ISBN-13: 978-0486652429, ISBN-10: 0486652424.
- “*Statistical Mechanics*”, by R K Pathria and Paul D. Beale, Academic Press, February 2011, 3rd Edition, ISBN: 9780123821881.
- “*Statistical Mechanics: Theory and Molecular Simulation*”, by Mark Tuckerman, Oxford University Press, 2011, ISBN: 9780198525264.

### Some Points to Keep in Mind.

1. **Learning is your responsibility.** This is a graduate level course and you must take responsibility to deeply understand the subject. Pay utmost attention during lectures, and keep up with the reading materials. Don't be shy, ask questions during lectures or after lectures. Please remember engaging is the best way to learn.
2. **Homework Problems.** First try working the homework problems independently. If you have difficulty moving forward even after several tries, please ask for help either from me during office hours or from TA's or from your peers. I encourage you to discuss homework problems in groups but when you sit down to finally write your homework, it should be done independently; and it should reflect your understanding of the problem.
3. **Grade is Just a Number.** Don't get into the race of just getting grades. Your aim should be to learn, understand, and master the subject. This requires a painful struggle through lectures, texts, and homeworks. Everyone has different backgrounds and has different speeds of learning; so invest the required time. Remember that: “Rome was not built in a day”.
4. **Think Critically and Challenge Yourself.** Critical thinking is possibly one of the most important skill that will help you in whatever you do in life. This course is an opportunity to develop that habit. Think critically about what you read and about homework problems. Don't be satisfied by just solving problems or understanding course contents. Challenge yourself to go beyond the class lectures and homework problems.

## Academic Dishonesty.

Please read the following carefully (taken from <https://www.winona.edu/business/96.asp>):

1. **Cheating:** Using or attempting to use unauthorized materials in any academic exercise or having someone else do work for you. Examples of cheating include looking at another student's paper during a test, bringing a crib sheet to a test, obtaining a copy of a test prior to the test date or submitting homework borrowed from another student.
2. **Deception and Misrepresentation:** Lying about or misrepresenting your work, academic records, or credentials. Examples of deception and misrepresentation include forging signatures, falsifying application credentials and misrepresenting group participation.
3. **Enabling Academic Dishonesty:** Helping someone else to commit an act of academic dishonesty. This would include giving someone else an academic assignment with the intent of allowing that person to copy it or allowing someone else to cheat from your test paper.
4. **Fabrication:** Refers to inventing or falsifying information. Examples of fabrication include drylabbing (inventing data) or making references to sources you did not use in academic assignments.
5. **Plagiarism:** Using the words or ideas of another writer without proper acknowledgement, so that they seem as if they are your own. Plagiarism includes behaviour such as copying someone else's work word for word, rewriting someone else's work with only minor word changes and/or summarizing someone else's work without acknowledging the source.

## Pledge

I, do solemnly promise that

1. I will maintain the highest standards of academic honesty during this course.
2. I have carefully read above forms of academic dishonesty and I will not indulge in any of them. If I am caught indulging in any one of them, I deserve one and only one grade, i.e., F.
3. I will maintain at least 90% of attendance during the discussion hours.

*"Try not be a person of SUCCESS but rather try to become a person of VALUE" — Albert Einstein*