MSE 6411 – Thermodynamics of Materials

Course Objective	To provide students with a fundamental understanding of the classical thermodynamics and statistical thermodynamics that govern the behavior of all materials in all states.
Learning Objectives	Upon completion of this course, students will be able to: (1) Understand the role of internal energy, entropy, and free energy in various chemical and physical material processes and for equilibrium/non-equilibrium states (2) Reduce thermodynamic aspects to the general framework of statistical mechanics (3) Acquire a thorough insight on a comprehensive approach to describe the behavior of assemblies of small molecules and long chain polymer molecules using classical thermodynamics and statistical thermodynamics (4) Apply thermodynamics approaches to understand behavior of surfaces and interfaces in materials
Academic Integrity	Students are reminded of the Georgia Tech Academic Honor Code and Student Code of Conduct. Academic dishonesty and violations of the Honor Code will be handled according to the established Georgia Tech policies. If specific polices described for tests and homework are not clear, students should clarify those with the instructors to assure proper compliance with expected policies.
Learning Accommodations	Proper accommodation will be provided, in accordance with Georgia Tech's policies, for students with documented disabilities that could affect their performance. Students should inform the instructor at the beginning of the semester if they are seeking such an accommodation.
Lectures	12:20 -1:10 pm M, W, F
Instructors	Arun Gokhale (lead instructor), Karl Jacob, and Robert Speyer
Teaching Assistants	Lei Zhang
Homework	Problems will be assigned periodically and solutions will be posted a week later. Homework may not be collected or graded
Exam/grading	4 Exams, 25% each at the end of each Part

Text books/References books

1. *Molecular Driving Forces – Statistical Thermodynamics in Chemistry and Biology*, by Ken A. Dill and Sarina Bromberg, Garland Science, Taylor & Francis Group, 2nd Edition.
2. *Thermodynamics in Materials Science* by Robert DeHoff, CRC, Taylor & Francis Group, 2nd Edition

TOPICS

PART I (Prof. Arun Gokhale)
Mathematics, probabilities, and statistics background, Laws of thermodynamics, Maxwell's relationships, liquid and solid solutions, chemical potential, conditions of equilibrium, phase diagrams, thermodynamics of reacting systems, Statistical Thermodynamics: Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics, Partition Function, Ensembles, Calculation of Thermodynamic functions from Partition Function, Einstein and Debye theories of heat capacity

PART II (Prof. Karl Jacob)

1. Continuum Fluids: Thermodynamics, Structure
    A. Hard Sphere Fluids (relevant to atoms, molecules, colloids)
        1-dimensional Tonks model, comparison to lattice fluid model
    B. Correlation functions, Radial Distribution Function g(r)
2. Solutions of long chain molecules and blends
    A. Flory-Huggins approach: effect of enthalpy, entropy and degree of polymerization
    B. UCST and LCST behavior

PART III (Prof. Robert Speyer)
Thermodynamics of point defects, surfaces and interfaces, Physical Adsorption, Monolayers and Langmuir Isotherm