



Course Syllabus: Chemical Thermodynamics - CE 201

Division	Physical Science and Engineering Division
Course Number	CE 201
Course Title	Chemical Thermodynamics
Academic Semester	Fall
Academic Year	2019/2020
Semester Start Date	08/25/2019
Semester End Date	12/10/2019
Class Schedule (Days & Time)	09:00 AM - 10:30 AM Mon Thu

Instructor(s)				
Name	Email	Phone	Office Location	Office Hours
Subram Maniam Sarathy	Mani.Sarathy@kaust.edu.sa	+966128084626	4222, 5, Al-Kindi (bldg. 5)	
Jorge Gascon Sabate	JORGE.GASCON@KAUST.EDU.SA	+966128080723	4235, 3, Ibn Sina (bldg. 3)	
Pedro Castano	pedro.castano@kaust.edu.sa	+966128087324	4276, 3, Ibn Sina (bldg. 3)	

Teaching Assistant(s)	
Name	Email

Course Information	
Comprehensive Course Description	The primary goal of chemical thermodynamics is the physical explanation of the fundamental principles governing the variety of chemical phenomena taking place in the world around us. The goal of this course is to give students a conceptual understanding of the main principles of thermodynamics. Topics include: the concept of entropy; the Clausius, Gibbs, Boltzmann and Shannon definition of entropy; entropy and information; Maxwells demon; the Boltzmann distribution law; the Maxwell-Boltzmann speed distribution; Gibbs and Helmholtz free energy; the chemical potential; Gibbs-Duhem and Euler equation; the Gibbs phase rule; entropy of mixing and Gibbs paradox; phase diagrams, the Flory-Huggins phase diagram; spontaneous and non-spontaneous processes; thermodynamics of chemical reactions; thermodynamics of osmosis and reverse osmosis, entropy and irreversible phase transitions; introduction in thermodynamics of irreversible processes; introduction in statistical thermodynamics; biological evolution, entropy and information
Course Description from Program Guide	The primary goal of chemical thermodynamics is the physical explanation of the fundamental principles governing the variety of chemical phenomena taking place in the work around us. The goal of this course is to give students a conceptual understanding of the main principles of thermodynamics. Topics include: the concept of entropy; the Clausius, Gibbs, Boltzmann and Shannon definition of entropy; entropy and information; Maxwells demon; the Boltzmann distribution law; the Maxwell-Boltzmann speed distribution; Gibbs and Helmholtz free energy; the chemical potential; Gibbs-Duhem and Euler equation; the Gibbs phase rule; entropy of mixing and Gibbs paradox; phase diagrams, the Flory- Huggins phase diagram; spontaneous and non-spontaneous processes; thermodynamics of chemical reactions; thermodynamics of osmosis and reverse osmosis, entropy and irreversible phase transitions; introduction in thermodynamics of irreversible processes; introduction in statistical thermodynamics;

Goals and Objectives	<p>The goal of this course is to give students a conceptual understanding of the main principles of thermodynamics.</p> <p>the concept of entropy will be discussed in detail; Students will learn the Clausius, Gibbs, Boltzmann and Shannon definition of entropy; relation entropy and information will be discussed; Students will learn about Maxwells demon, the Boltzmann distribution law, the Maxwell-Boltzmann speed distribution, Gibbs and Helmholtz free energy, the chemical potential, the Gibbs-Duhem and Euler equation, the Gibbs phase rule; entropy of mixing and Gibbs paradox; phase diagrams, the Flory-Huggins phase diagram; spontaneous and non-spontaneous processes; thermodynamics of chemical reactions; thermodynamics of osmosis and reverse osmosis, entropy and irreversible phase transitions; introduction in thermodynamics of irreversible processes; students will learn the basics of statistical thermodynamics;</p>
Required Knowledge	An undergraduate thermodynamic course
Reference Texts	<p>REQUIRED TEXT : Atkins' Physical Chemistry</p> <p>REFERENCE TEXTS : E. Fermi, Thermodynamics</p> <p>Henry A. Bent, An introduction to classical and statistical thermodynamics</p> <p>Mikhail V. Volkenstein, Entropy and Information</p>
Method of evaluation	<p>35.00% - Exam 1</p> <p>30.00% - Homework /Assignments</p> <p>35.00% - Exam 2</p>
Nature of the assignments	2 homeworks (maximum points 15 per homework), mid-term exam (max. points 35), final exam (max. points 35)
Course Policies	In accordance with the University policy and professional standards, the highest levels of academic integrity are expected in this class. The code of student conduct is strictly enforced. Academic dishonesty will result in reductions in grades and/or expulsions from this class and/or the University.
Additional Information	

Tentative Course Schedule

(Time, topic/emphasis & resources)

Week	Lectures	Topic
1	Mon 08/26/2019	Intro + first law
1	Thu 08/29/2019	Enthalpy, Joule Thomson effect
2	Mon 09/02/2019	Exercises & Entropy & The second law
2	Thu 09/05/2019	Entropy and The second law
3	Mon 09/09/2019	Spontaneous and non spontaneous processes
3	Thu 09/12/2019	Helmholtz and Gibbs free energy + Exercises
4	Mon 09/16/2019	Exercises + Variation of Gibbs free energy with temperature and pressure + Phase diagrams
4	Thu 09/19/2019	Simple mixtures and chemical potential
5	Mon 09/23/2019	Saudi National Day
5	Thu 09/26/2019	Solvent and solute activity
6	Mon 09/30/2019	Solvent and solute activity
6	Thu 10/03/2019	Thermodynamics of chemical reactions
7	Mon 10/07/2019	Chemical reactions
7	Thu 10/10/2019	Exercises
8	Mon 10/14/2019	Assignment solutions
8	Thu 10/17/2019	Intro to quantum mechanics
9	Mon 10/21/2019	heat capacities, Einstein solid,
9	Thu 10/24/2019	Dynamics of microscopic systems - Schrodinger equation and Born approximation
10	Mon 10/28/2019	Mid-semester break
10	Thu 10/31/2019	Quantum theory of motion - Translation
11	Mon 11/04/2019	Midterm review
11	Thu 11/07/2019	Midterm Exam
12	Mon 11/11/2019	Quantum theory of motion - Vibrations and Rotation
12	Thu 11/14/2019	Molecular Spectroscopy - Rotational spectroscopy
13	Mon 11/18/2019	Molecular Spectroscopy - Vibrational spectroscopy
13	Thu 11/21/2019	Statistical Thermodynamics - Boltzmann Distribution
14	Mon 11/25/2019	Statistical Thermodynamics - Partition Functions
14	Thu 11/28/2019	Flory Huggins phase diagram
15	Mon 12/02/2019	Thermodynamics quantitative structure property relationships (QSPR) and machine learning
15	Thu 12/05/2019	Exercises and exam review
16	Mon 12/09/2019	Exams

Note

The instructor reserves the right to make changes to this syllabus as necessary.