Lahore University of Management Sciences

ChE513 - Electrochemical Energy Systems

CHEM 513- Electrochemical Energy Storage & Conversion

Spring 2024

Instructor	Ali Rauf
Room No.	9-445A
Office Hours	TBD
Email	ali.rauf@lums.edu.pk
Telephone	3560-8281
Secretary/TA	TBD
TA Office Hours	TBD
Course URL (if any)	-

Course Teaching Methodology (Please mention following details in plain text)

- On campus classes

Course Basics				
Credit Hours	3			
Lecture(s)	Nbr of Lec(s) Per Week	2	Duration	75 min
Recitation (per week)	Nbr of Rec (s) Per Week	-	Duration	-
Lab (if any) per week	Nbr of Session(s) Per Week		Duration	
Tutorial (per week)	Nbr of Tut(s) Per Week	-	Duration	

Course Distribution	
Core	
Elective	-
Open for Student Category	SBASSE Chemistry Senior, MS and PHD students, EE MS and PhD students, ChE PhD Students
Closed for Student Category	Non Chemistry Majors

COURSE DESCRIPTION

Energy is a fundamental issue facing society world-wide. Electrochemical devices play an important role in energy storage and conversion, especially at certain power-levels. Evolving renewable energy sources have a critical dependence on electrochemical energy storage. The hydrogen economy depends on electrochemical devices for hydrogen production (i.e., electrolyzes) and conversion (i.e., fuel cells).All electrochemical devices (e.g., electrolyzes, fuel cells and batteries) are based on fundamental electrochemical principles. These electrochemical principles are derived from

a) Thermodynamics

b) Kinetics

c) mass transport

In the first half of the course, the students learn the 'fundamentals of electrochemistry'. This involves applying their previous knowledge of thermodynamics, kinetics, and transport to electrochemical systems. **In the second half of the course, the fundamental of electrochemistry are applied to specific electrolyzes including water/CO_2 electrolyzes and capacitors.** Practical aspects of these systems, such as performance metrics, safety, and wear-out mechanisms are also presented. The students can explore aspects of electrochemical systems of particular interest to them in more depth.

Course Project

An independent/ group study project based on analysis of electrochemical energy system will be an integral part of this course where students acquire more depth on a particular aspect of their choosing energy system. The formal written report will constitute a significant part of overall grade. All reports will be shared with the full class.

COURSE PREREQUISITE(S)	
•	CHEM 101

Learning Outcomes	
	CLO-1: Understand how thermodynamics, kinetics and mass transport apply to electrochemical devices. **CLO-2: Evaluate** the fundamental electrochemical properties of electrodes by using electrochemical techniques. **CLO-3: Analyze** the performance of energy storage and conversion devices derived from fundamental thermodynamic, kinetic and Transport principles.

Grading Breakup and Policy

Quiz(s): 15% (5-6)

Homework: 10%

Midterm Examination: 30%

Final Project: 10%

Final Examination: 35%

Attendance Policy:
All Students need to ensure minimum 75% attendance in this course. Otherwise, you may get F or a two grade reduction based on case by case policy.

Examination Detail	
Midterm Exam	Yes/No: Yes Combine Separate: NA Duration: 75 min Preferred Date: NA Exam Specifications: NA

Final Exam	Yes/No: Yes Combine Separate: NA Duration: 3 hrs Exam Specifications: NA

Course Overview			
Week	Topic	Recommended Readings	Related CLO
1a	**Introduction and Basic Principles** a) Importance of electrochemical systems and its Examples b) Electrochemical cells c) Scientific units, Constants and Conventions d) Faraday's Laws e) Potential and Ohm's Law	Textbook: EE (Chapter 1, Pages 1-12)	CLO1
1b	**Cell Potential And Thermodynamics** a) Electrochemical Reactions and their Characteristics b) Gibbs Free Energy and Cell Potential and its expression c) Nernst Equation d) Standard Potential and Effect of temperature on it	Textbook: EE (Chapter 2, Section 2.1-2.5, Pages 15-22)	CLO1
2a	**Cell Potential And Thermodynamics (cont...)** a) Use of cell Potential b) Equilibrium Constant c) Pourbaix Diagrams d) Cells with Liquid Junctions and Reference Electrodes e) Equilibrium at electrode Interface	Textbook: EE (Chapter 2, Section 2.7-2.12, Pages 24-31)	CLO1
2b	**Cell Potential And Thermodynamics (cont...)** a) Debye-Huckel Theory b) Activity and activity coefficients c) Estimation of Activity coefficient d) Electrode Cell Setup	Textbook: EE (Chapter 2, Section 2.13-2.15, Pages 31-36)	CLO1
3a	**Electrochemical Kinetics** a) Electrode Solution Interface (Double Layer) b) Relationship b/w Current and Rate constant c) Impact of potential on rate constant (derivation of Butler Volmer Kinetic Expression) d) *Relationship b/w Potential and Energy Barriers*	Textbook: EE (Chapter 3, Section 3.1-3.2, Pages 41-46) ***And Instructor Notes***	CLO1
3b	**Electrochemical Kinetics (cont...)** a) Uses/Implications of Butler-Volmer Kinetic Expression 1. Charge Transfer overpotential 2. Exchange Current density b) Simplified forms of Butler Volmer Equation c)Direct Fitting of the Butler Volmer Equation	Textbook: EE (Chapter 3, Section 3.3-3.6, Pages 46-54)	CLO1

4a	**Electrochemical Kinetics (cont...)** a) Effect of mass transfer on the reaction rate b) Use of Kinetic Expressions in Full Cells c) Current Efficiency	Textbook: EE (Chapter 3, Section 3.7-3.9 Pages 46-58)	CLO1
4b	**Transport** a) Types of Mass Transfer and Nernst-Planck Equation b) Conservation of material *c) Migration* *d) Mixed Migration and diffusion near active electrode*	Textbook: EE (Chapter 4, Section 4.1-4.3 Pages 63-71) ***And Instructor Notes***	CLO1
5a	**Transport (cont...)** a) Transference Number, Mobilities and Migration b) Diffusion and Fick's Law c) Convective Mass Transport	Textbook: EE (Chapter 4, Section 4.4-4.5 Pages 71-79)	CLO1
5b	**Transport (cont...)** a) Concentration Overpotential b) Current Distribution c) Membrane Transport	Textbook: EE (Chapter 4, Section 4.6-4.8 Pages 79-87)	CLO1
6a	**Electrochemical Energy Storage: Battery Fundamentals** a) Component of a cell b) Classification of Batteries and Cell Chemistries c) Theoretical Capacity, state of Charge, Charge retention and Self Discharge	Textbook: EE (Chapter 7, Section 7.1-7.3 Pages 151-158)	CLO3
6b	**Electrochemical Energy Storage: Battery Fundamentals (cont...)** d) Cell Characteristic and Electrochemical Performance e) Ragone Plot f) Heat Generation g) Efficiency of secondary cell	Textbook: EE (Chapter 7, Section 7.4-7.9 Pages 158-168)	CLO3
7a	**Electrochemical Energy Storage: Capacitors Fundamentals** a) Introduction and brief overview on history of supercapacitors b) Comparison among various Electrochemical energy storage devices c) Components of Supercapacitors d) Classification of supercapacitors based on charge storage mechanism e) Supercapacitors Principles f) Method for supercapacitor Evaluation	***Instructor Notes***	CLO3
7b	***Midterm***		

8a	**Electrochemical energy Conversion** **H_2O Electrolyzers Fundamentals** a) Importance of water electrolysis in energy storage and conversion b) Brief introduction of water Electrolyzers c) Fundamentals of water electrolysis	***Instructor Notes***	CLO3
8b	**Electrochemical energy Conversion** **CO_2 Electrolyzers Fundamentals** a) Chemical and physical properties of CO_2 and its electro reduction b) Thermodynamics of CO_2 electroreduction c) Factors affecting Electrochemical reduction of CO_2 d) Electrode kinetics of CO_2 electroreduction e) Mechanism of Electroreduction and Product Selective production of Different reduced products	***Instructor Notes***	CLO3
9a 9b 10a	**Electroanalytical Techniques and Analysis of Electrochemical Systems:** **Sweep Voltametric Techniques** a) Introduction b) Linear Sweep Voltammetry c) Cyclic Voltammetry its basics and fundamentals d) Cyclic voltammograms of Reversible, Quasi Reversible, Irreversible Processes e) Effect of Homogenous Chemical reactions f) Effects due to electrode type, Resistance, geometry, sizes and Convection **Electroanalytical Techniques and Analysis of Electrochemical Systems:** **Pulse Voltammetry** a) Introduction b) Polarography and its fundamental Equation c) Different Types of Voltammetry (staircase, Normal Pulse, Reverse Pulse, Differential Pulse and Square-wave Voltammetry)	Reference Book 1: TEC (Chapter 2, Section 2.1-2.4) Reference Book 1: TEC (Chapter 3, Section 3.1-3.8)	CLO2
10b	**Electroanalytical Techniques and Analysis of Electrochemical Systems:** **Chronoamperometry** a) Introduction and fundamental concepts b) Experimental setup for CA c) Practical Problems and Applications d) Examples of CA Applications in research	Reference Book 1: TEC (Chapter 4, Section 4.1-4.4)	CLO2
11a	**Lab Activity**		
11b 12a	**Electroanalytical Techniques and Analysis of Electrochemical Systems:** **Electrochemical Impudence**	Textbook: EE (Chapter 6, Section 6.7 Pages 129-136)	CLO2
12b	**Lab Activity**		

13a	**How properly are we interpreting the Tafel lines in energy conversion electrocatalysis?** a) Tafel Analysis an overview b) What does Tafel Analysis offer us c) Do and Don's in Tafel Analysis	Review Article	CLO2
13b	**iR drop correction in electrocatalysis: everything one needs to know!** a) Factors Influencing iR drop b) iR drop correction c) Challenges and best practices	Textbook: EE (Chapter 6, Section 6.7 Pages 139-141) & Review Article	CLO2
14a	**Dos and Don'ts in Screening Water Splitting Electrocatalysts** a) Methods and parameters of evaluation an overview b) Systematic use of electroanalytical techniques in screening H2O splitting electrocatalyst c) Assessing activity d) Apparent activity markers e) Assessing Selectivity f) Assessing Stability g) Miscellaneous Supporting studies	Review Article	CLO2
14b	**Precision and correctness in the evaluation of electrocatalytic water splitting: revisiting activity parameters with a critical assessment** a) Overpotential and its importance b) Tafel Analysis and Exchange current density c) Mass and Specific activity d) TOF e) Is ECSA an activity parameter f) Screening an electrocatalyst for Stability and endurance in H2O splitting electrocatalysis best practices	Review Article	CLO2
16	Final Exam		

Textbook(s)/Supplementary Readings

Textbook

1. Electrochemical Engineering, Thomas F. Fuller and John N. Harb, 2018, John Wiley & Sons, Inc, Hoboken NJ. ISBN: 978-1-119-00425-7.

Reference Books

1. Techniques in Electroanalytical Chemistry by Olia simoska & Shelley D. Minteer https://pubs.acs.org/doi/epub/10.1021/acsinfocus.7e5021
2. Electrochemical methods Fundamentals and applications, Allen J. Bard and Larry R. Faulkner, 2002, John Wiley & Sons, Inc, ISBN 0-471-04372-9.