UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

# COURSE SYLLABUS

## Models and Materials for Electrochemical Energy Generation and Conversion

**2324-1-FSM01Q018**

### Aims

The course aims to provide the students with knowledge related to the electrochemical systems for energy generation and conversion including materials and their synthesis processes and device applications. With this course, the materials (classification, synthesis and integration) used in electrochemical devices such as fuel cells, electrolyzers and bioelectrochemical systems will be presented. Within the course, catalysis and electrocatalysis aspects, transport phenomena occurring on the electrodes, electrochemical processes, electrodes and electrolyte fabrication methods and integration, technological operation and electrochemical performance will be evaluated.

### Contents

Catalysis and electrocatalysis. Electrochemical technologies for energy conversion and generation. Water electrolyzers, fuel cells, carbon dioxide reduction, bioelectrochemical systems.

### Detailed program

From thermal catalysis to electrocatalysis: short recall of fundamental theoretical aspects in heterogeneous catalysis, and electrocatalysis: reaction kinetics, mechanism, barriers, and overpotential.

What is the actual catalyst? The interplay between experiments and modelling in characterizing the structural and chemical features of the catalyst: definition of the active site, morphological and chemical characterization of the active species by means of microscopic and spectroscopic techniques and theoretical modelling.

Electrocatalysis at work: rationalization of the activity trends in oxygen reduction reaction, water splitting, hydrogen evolution reaction, oxygen evolution reaction, CO2 electroreduction: reaction mechanisms, expected activity, pros and cons of various electrocatalysts.
From nanoparticles to single atoms: the size aspect of a catalyst. A critical overview on the usage of highly dispersed catalytic species.

Water Electrolyzers. Classification of electrolyzers (AEL, PEMEL, AEMEL, SOEC, CO2 electrolyzers). Strategies to optimize the reaction pathways (hydrogen evolution reaction, oxygen evolution reaction, CO2 electroreduction). Identification of performance, polarization curves, losses, durability issues. Effect of operational parameters (e.g. T, P) on the electrochemistry. Organic, inorganic and hybrid materials for electrocatalysts and membranes. Fabrication of electrocatalysts architectures, polymeric membranes and their integration in membrane electrode assembly. Identification of gaps and proposed solutions. Substitution of critical raw materials (e.g. Pt, Ir and Co) and fluorinated compounds. Device operations.

Fuel Cells. Classification of fuel cells operating with gaseous feedstock (PEMFC, AEMFC, AFC, MCFC, SOFC) and liquid feedstock (DMFC, DEFC, DFAFC, etc). Strategies to optimize the reaction pathways (hydrogen oxidation reaction, alcohol oxidation reaction, oxygen reduction reaction). Identification of performance, polarization curves, losses, durability issues. Effect of operational parameters (e.g. T, P, etc) on the electrochemistry. Organic, inorganic and hybrid materials for electrocatalysts and membranes. Fabrication of electrocatalysts architectures, polymeric membranes and their integration in membrane electrode assembly. Identification of gaps and proposed solutions. Substitution of critical raw materials (e.g. Pt and Co) and fluorinated compounds. Device operations

Bioelectrochemical systems. Classification of bioelectrochemical systems (MFC, MEC, MDC, EFC, etc). Interaction bacterial-surface or enzyme-surface. Modification of surface for enhancing/decrease bacterial/enzyme attachment. Reaction mechanisms of microorganisms and enzymes (bacterial and enzymatic). Identification of gaps and proposed solutions. Device operations

Application of electrochemical devices. The course will be completed with a discussion on the devices at the state of the art in the different sectors on interest such as automotive, residential, and industrial giving a roadmap towards the EU goal of decarbonization in 2050.

## Prerequisites

Standard physic and mathematic knowledge, thermodynamic and kinetic of chemical systems.
Suggested: Fundamentals of Electrochemistry for Energy Storage

## Teaching form

Face to face

## Textbook and teaching resource

Teacher's slides and selected chapters from the following books:
• Selected scientific papers and reviews
• Bard Faulkner: Electrochemical Methods, Fundamental and Applications (2° Edition)
• IRENA Report (IRENA (2020), Green Hydrogen Cost Reduction: Scaling up Electrolysers to Meet the 1.5oC

Climate Goal, International Renewable Energy Agency, Abu Dhabi)
• Fuller and Harb, Electrochemical Engineering, Wiley 2018
• Pei Kang Shen, Chao-Yang Wang, San Ping Jiang, Xueliang Sun, Jiujun Zhang. Electrochemical Energy Advanced Materials and Technologies. 2017. CRC Press
• F. Marken, D. Fermin. Electrochemical Reduction of Carbon Dioxide: Overcoming the Limitations of Photosynthesis. RSC Publishing. 2018
• S. Cosnier. Bioelectrochemistry: Design and Applications of Biomaterials. Publisher: De Gruyter. Edited by Serge Cosnier. ISBN 978-3-11-056898-1. DOI : 10.1515/9783110570526-010
• Xu, Kang "Electrolytes, Interfaces and Interphases Fundamentals and Applications in Batteries", RSC Publishing

## Semester

Second Semester (entire semester)

## Assessment method

Research project on a topic related to the course. (50%)
Oral presentation at the end of the course. (50%)

## Office hours

On appointment contacting the Lecturer via email.

## Sustainable Development Goals

AFFORDABLE AND CLEAN ENERGY