

# UNIVERSITÀ DEGLI STUDI DI MILANO-BICOCCA

# SYLLABUS DEL CORSO

# Models and Materials for Electrochemical Energy Generation and Conversion

2526-1-FSM02Q018

#### **Aims**

The course aims to provide students with the principles and of electrochemical technologies for energy conversion, and to place them in the broader context of the current energy scenario.

#### Knowledge and understanding

At the end of the course, the student will know:

Basic concepts of electrochemical conversion systems (electrolytes, electrodes, their integration into membrane electrode assembly).

Main technologies for electrochemical energy conversion including fuelc ells and electrolyzers and novel conversion systems such as carbon dioxide conversion and nitrate reduction

Materials and operations of electrochemical energy conversion systems.

Effect of operating parameters (e.g. temperature and pressure) on the performance.

#### Applying knowledge and understanding

At the end of the course, the student will be able to:

Identify the main components of fuel cells and water electrolyzers.

Apply the knowledge for selection of materials.

Apply the acquired knowledge to critically evaluate the choice of materials in different electrochemical energy conversion devices, considering their structural, electronic and functional properties.

Assemble an electrochemical conversion device, selecting electrolytes and electrode materials.

Understand the polarization curves and analyses on the various components of the system (membrane separator, anode and cathode)

#### **Making judgments**

At the end of this course, the student must demonstrate the ability to:

Demonstrate mastery of the topics covered in the course

Understand the operating principle of an electrochemical energy storage device

Demonstrate the ability to critically analyze electrochemical data collected in the laboratory. This also includes the

ability to organize the data in a scientific paper.

#### **Communication skills**

At the end of this activity, the student will be able to orally and with proper language skills present the scientific topics related to energy conversion systems. The student will also be able to produce a written paper related to the laboratory experiments.

#### Learning skills

Upon completion of the course, the student is able to:

Independently deepen their knowledge of electrochemical energy conversion materials and devices through existing scientific literature.

Constantly update themselves on research developments and technological evolution in the field of electrochemical conversion systems including the substitution of critical raw materials with less noble and precious materials.

Critically evaluate information and data and finally support decision-making and problem solving.

Develop a multidisciplinary (materials science, chemistry and engineering) and multiscale (from atomic level to system level) approach to the study and understanding of electrochemical energy conversion systems.

Effectively continue their learning path both in academic and professional settings, particularly in the field of energy conversion technologies.

#### **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**

16 two-hour lectures, in person, Delivered Didactics12 two-hour practical classes, in person, Interactive Teaching

# 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

Presentation of a review article at the end of the course.

There are no intermediate ongoing tests.

The presentation method, knowledge of the topic and ability to answer questions will be assessed.

Furthermore, the skills acquired during the course will be evaluated.

## Office hours

On appointment contacting the Lecturers via email.

# **Sustainable Development Goals**

AFFORDABLE AND CLEAN ENERGY