

PhD COURSE DESCRIPTION

Course title	Field of science, code	Faculty / Center	Department
Electrochemical Energy Conversion Systems	Chemistry N 003	FTMC	Chemical Engineering and Technologies
Student's workload	Credits	Student's workload	Credits
Lectures	2	Consultations	0
Independent study	6	Seminars	2

Course description

Course summary:

This advanced course provides an in-depth coverage of the principles and applications of electrochemical processes for energy conversion and storage. The topics include thermodynamics, kinetics, mass and charge transport in electrochemical systems. The applications and energy conversion systems, such as fuel and electrolysis cells, photoelectrochemical cells, batteries, and hybrid systems, will be discussed. The course aims to provide PhD students with the knowledge necessary for careers in research.

Course contents:

1. Cell Thermodynamics and Potentials
 - a) Electrochemical thermodynamics
 - b) Equilibrium and electrochemical potentials
 - c) Interfacial potentials
 - d) Junction potentials
 - e) Formal potentials and reference electrodes
 - f) Temperature and pressure dependence
2. Electric Double Layer
 - a) Ideally polarizable electrodes
 - b) Models of the electric double layer
 - a) Specific adsorption
 - b) Double layer effects on reaction kinetics
3. Electrode Kinetics
 - a) Phenomenological Butler-Vollmer kinetics
 - b) Microscopic Marcus theory
 - c) Multi-step reactions
4. Electrokinetic and Electrocapillary Phenomena
 - a) Electroosmosis
 - b) Electrophoresis
 - c) Electrocapillary motion
5. Thermodynamics and Transport in Electrolyte Solutions
 - a) Activities
 - b) Dilute electrolytes and Debye-Hückel theory
 - c) Transport laws
 - d) Diffusion, conductivity, transference numbers
 - e) Concentrated electrolytes
6. Transport in Solid State
 - a) Equilibrium thermodynamics in real solids
 - b) Irreversible thermodynamics and kinetics in solids
 - c) Phenomenological diffusion coefficients
 - d) Charge mobility
 - e) Concentration profiles
7. Mass and Charge Transfer in Electrochemical Systems
 - a) Mass transfer equations
 - b) Electroneutrality
 - c) Migration and diffusion at the electrode surface
 - d) Convective transport
 - e) Concentration overpotential
8. Porous Electrodes
 - a) Microscopic description

- b) Mass transfer
 - c) Reaction rate non-uniformity
 - d) Applied aspects
- 9. Electrochemical Impedance
 - a) Equivalent AC circuits
 - b) Kramers-Kronig relations
 - c) Instrumentation
 - d) Physical modeling
- 10. Photoelectrochemistry
 - a) Semiconductor-electrolyte junction
 - b) Photoelectrochemical cells
 - c) Surface photocatalysis
 - d) Electrochemiluminescence and electrochromism
- 11. Ion Insertion Systems
 - a) Binary and tertiary electrodes near equilibrium
 - b) Redox and insertion reaction potentials
 - c) Single- and two-phase reactions
 - d) Types of insertion electrodes
- 12. Ion Batteries
 - a) Ion insertion battery materials and systems
 - b) Electrode conversion (alloying) battery materials and systems
 - c) Applied aspects of electrochemical batteries
- 13. Flow Batteries
 - a) Flow battery structure and components
 - b) Redox and redox-mediated processes
 - c) Applied aspects of flow batteries
- 14. Fuel and Electrolysis Cells
 - a) Classification of fuel and electrolysis cells
 - b) Structure and components
 - c) Electrocatalysis
 - d) Electrolytes and membranes
 - e) High- and low-temperature systems
- 15. Hybrid Electrochemical Energy Conversion Systems
 - a) Electric double layer capacitors
 - b) Pseudocapacitance and supercapacitors
 - c) Applied aspects of hybrid energy conversion systems
- 16. Additional aspects of electrochemical energy conversion
 - a) Biological electrochemical energy conversion systems
 - b) Techno-economics of electrochemical energy conversion

References

1. Newman, John, and Balsara, Nitash P. *Electrochemical systems*. John Wiley & Sons, 2021.
2. Bockris, John O'M., Reddy, Amulya KN and Gamboa-Adelco, Maria E. *Modern Electrochemistry 1, 2A, and 2B*. Springer US, 2006.
3. Bard, Allen J., Faulkner, Larry R. and White, Henry S. *Electrochemical methods: fundamentals and applications*. John Wiley & Sons, 2022.
4. Hamann, Carl, Hamnett, Andrew and Vielstich, Wolf. *Electrochemistry*. John Wiley & Sons, 2007.
5. Bagotsky, Vladimir S., *Fundamentals of electrochemistry*. John Wiley & Sons, 2005.
6. Eliaz, Noam, and Gileadi, Eliezer. *Physical electrochemistry: fundamentals, techniques, and applications*. John Wiley & Sons, 2019.
7. Schmickler, Wolfgang, and Santos, Elizabeth. *Interfacial electrochemistry*. Springer Science & Business Media, 2010.
8. Hammou, Abdelkader, and Georges, Samuel. *Solid-state electrochemistry: essential course notes and solved exercises*. Springer Nature, 2020.
9. Bagotsky, Vladimir S., Skundin, Alexander M. and Volfkovich, Yuriy M. *Electrochemical power sources: batteries, fuel cells, and supercapacitors*. John Wiley & Sons, 2015.
10. Huggins, Robert. *Advanced batteries: materials science aspects*. Springer Science & Business Media, 2008.
11. Orazem, Mark E., and Tribollet, Bernard. *Electrochemical impedance spectroscopy*. John Wiley & Sons, 2017.
12. Dicks, Andrew L., and Rand, David AJ. *Fuel cell systems explained*. John Wiley & Sons, 2018.
13. O'Hayre, Ryan. *Fuel cell fundamentals*. John Wiley & Sons, 2016.
14. Memming, Rüdiger. *Semiconductor electrochemistry*. John Wiley & Sons, 2015.

15. Lewerenz, Hans-Joachim and Laurence, Peter. *Photoelectrochemical Water Splitting. Materials, Processes and Architectures*. RSC Publishing, 2013.
16. Gimenes, Sixto and Bisquert, Juan. *Photoelectrochemical Solar Fuel Production*. Springer, 2016.
17. Oldham, Keith, Myland, Jan and Bond, Alan. *Electrochemical science and technology: fundamentals and applications*. John Wiley & Sons, 2011.
18. Fuller, Thomas F. and Harb, John N. *Electrochemical engineering*. John Wiley & Sons, 2018.

Responsible people	Scientific degree	Key related scientific publications over the last 5 years
Linās Vilčiauskas Jurga Juodkazytė	Dr. Dr.	1. J Juodkazytė, B Šebeka, I Savickaja, M Petrulevičienė, S Butkutė, V Jasulaitienė, A Selskis, R Ramanauskas; Electrolytic splitting of saline water: Durable nickel oxide anode for selective oxygen evolution, <i>International Journal of Hydrogen Energy</i>, 44, 5929 (2019). 2. Pilipavičius, J.; Traškina, N.; Juodkazytė, J.; Vilčiauskas, L.; The mechanism of NaTi₂(PO₄)₃ aqueous electrochemical degradation revisited, <i>Electrochimica Acta</i>, 465, 142993 (2023). doi:10.1016/j.electacta.2023.142993 3. Petrulevičienė, M.; Traškina, N.; Pilipavičius, J.; Juodkazytė, J.; Vilčiauskas, L.; The Use of Reductive Agents for Developing Capacity Balanced Aqueous Sodium Ion Batteries, <i>Batteries & Supercapacitors</i>, 6, e202300129 (2023). doi:10.1002/batt.202300129 4. Petrulevičienė, M.; Pilipavičius, J.; Juodkazytė, J.; Gryaznov, D.; Vilčiauskas, L.; Electrochemical Performance of NASICON-structured Na_{3-x}V_{2-x}Ti_x(PO₄)₃ (0.0 < x < 1.0) as Aqueous Na-ion Battery Positive Electrodes, <i>Electrochimica Acta</i>, 424, 140580 (2022). doi:10.1016/j.electacta.2022.140580 5. Snarskis, G.; Pilipavičius, J.; Gryaznov, D.; Mikoliūnaitė, L.; Vilčiauskas, L.; Peculiarities of Phase Formation in Mn-Based Na Superionic Conductor (NaSiCon) Systems: The Case of Na_{1+2x}Mn_xTi_{2-x}(PO₄)₃ (0.0 ≤ x ≤ 1.5), <i>Chemistry of Materials</i>, 33, 8394 (2021). doi:10.1021/acs.chemmater.1c02775 6. Plečkaitytė, G.; Petrulevičienė, M.; Staišiūnas, L.; Tediashvili, D.; Pilipavičius, J.; Juodkazytė, J.; Vilčiauskas, L.; Understanding and mitigation of NaTi₂(PO₄)₃ degradation in aqueous Na-ion batteries, <i>Journal of Materials Chemistry A</i>, 9, 12670 (2021). doi:10.1039/D1TA01215K 7. Petrulėviciene, M., Savickaja, I., Grigučeviciene, A., Naujokaitis, A., Ramanauskas, R., Juodkazyte, J., Optimization of BiVO₄ coatings for high yield photoelectrochemical production of reactive chlorine species, <i>Journal of Photochemistry and Photobiology A: Chemistry</i>, 443, 114842 (2023). doi:10.1016/j.jphotochem.2023.114842

Certified during the Doctoral Committee session on March 3rd, 2025. Protocol No. 15600-KT-79.
Committee Chairman prof. habil. dr. Audrius Padarauskas.