Mini Course on Theoretical Electrochemistry

Dr Mathijs Janssen

Norwegian University of Life Sciences

June 9 – June 13, 2025 (Monday – Friday)

Registration deadline: June 2, 2025; send an e-mail to skondrat@ichf.edu.pl, panos@ifpan.edu.pl

This flash course focuses on modeling the charging of porous electrodes, with applications in energy storage and conversion. Over five lectures (each 2 × 45 minutes), we will explore how electrolytes interact with both flat and porous electrodes in response to temperature variations and applied electric fields. While the focus is on theoretical and mathematical modeling, each lecture will include connections to experiments and applications.

1. **Equilibrium electrolytes and the electrical double-layer near a flat electrode**. Gouy-Chapman, Stern, Bikerman, and Kornyshev models, and results from classical density functional theory (DFT) and molecular dynamics. *Suggested reading: Härtel et al. JPCM **27** (2015).*
2. **Electrical double-layer formation near flat electrodes**. I will discuss continuum methods like the Nernst-Planck equation (PNP) and recent dynamical DFT and molecular simulations. The lecture also contains a tutorial on how to solve PDEs with Laplace transformations. *Suggested reading: Bazant et al. PRE **70** (2004); Janssen and Bier, PRE **97** (2018); Ma et al. JCP **156** (2022)*
3. **Electrical double layer formation in porous electrodes.** Macroscopic porous electrode theory (Newman/Biesheuvel-Bazant) vs. pore scale modeling (de Levie + many others). Analytical and numerical solutions to the PNP equations to describe the charging of pores. Tutorial on electrochemical impedance spectroscopy. *Suggested reading: Pedersen et al. PRX Energy **2** (2023)*
4. **Energy harvesting using (porous) electrodes**. "Blue energy" harvesting from salinity differences between sea and riverwater. Capacitive deionization. Harvesting thermal energy by charging/discharging supercapacitors. *Suggested reading: Brogioli PRL **103** (2009), Härtel et al. EES **8**(2015), Janssen et al. J. Mol. Liq. **371** (2023).*
5. **Interplay between temperature and ionic charge in electrolytes.** When a gas is compressed adiabatically its temperature rises— theory and experiments show that a similar reversible temperature effect also occurs when electric double layers form. I will also discuss the "electrolyte Seebeck effect": the electric field generated by an electrolyte in a thermal gradient. *Suggested reading: Janssen et al. PRL **118** & **119** (2017); Nickel et al. PRL **132** (2024)*

Level/Prerequisites: The course is meant for advanced undergraduate and graduate students, as well as researchers in electrochemistry and physical chemistry. You will get most out of it if you have previously taken at least introductory courses in electrodynamics, thermodynamics, statistical physics, and differential equations.