

Wolfson Department of Chemical Engineering Seminar

Monday, December 9th, 2024, at 13:30, Hall 6

Evaluation of the Oxygen Evolution Reaction Kinetics of Ni-based Electro-catalysts by Distribution Function of Relaxation Times Modelling

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Water splitting is a sustainable approach for converting electrical energy to chemical energy without CO₂ emission at the site. Two half-cell reactions occur during the water-splitting process: (i) oxygen evolution reaction (OER) and (ii) hydrogen evolution reaction (HER). OER is the major bottleneck due to several reaction steps in transferring the required four electrons, and slowing down the reaction kinetics. Thus, developing an efficient catalyst that executes the reaction at a low overpotential and exhibits good stability is desirable. The first part of this study focuses on a new strategy to optimize nickel-based oxy/hydroxide catalysts exhibiting high catalytic activity in alkaline solutions for OER. However, one of the main issues in the optimization process is the kinetics evaluation of electrocatalysts. The classic method to evaluate the reaction kinetics of electrochemical processes is based on the Tafel equation. Although the Tafel slope is an easy analytical technique, it is often imprecise and may lead to confusion about the catalyst's capabilities. The main goal of this work is to suggest a better way to get the information provided by a Tafel slope using the effective resistance Tafel equation. Our strategy applies electrochemical impedance spectroscopy (EIS) to identify the electrochemical phenomena at the catalyst/electrolyte interface. Instead of using equivalent circuit (EC) modeling, we run MATLAB-based genetic programming software, ISGP, to analyze and extract physical information from EIS. ISGP provides an analytical form of the distribution function of relaxation times (DFRT), allowing the extraction of the effective resistance and capacitance of each electrochemical phenomenon. The advantage is the ability to identify and separate Faradaic from non-Faradaic processes.

Therefore, in the second part of the study, we selected RuO₂, a benchmark catalyst, to serve as a reference for investigating the reaction kinetics using classical and effective resistance methodologies. After demonstrating that the ISGP method can enhance analysis or be more effective than classical Tafel slope analysis in certain situations, we applied the same procedure to examine the kinetics of our synthesized catalyst, nickel-based oxy/hydroxide.

The last part focuses on the Anion Exchange Membrane Water Electrolyzer (AEMWE), which sparked increased activity in the fundamental scientific aspects of technology. We expand our ISGP methodology to AEMWE to identify and quantify the different resistances contributing to cell performance losses. We examined the effects of KOH concentration in the electrolyte, electrolyte feeding configuration with different electrolytes, operating temperature, and various membrane types on the performance of AEMWEs. This analysis aims to enhance understanding of AEMWE loss sources to promote advancements in hydrogen production.

Refreshments will be served at 13:15