Intitulé du Sujet de Thèse : … Étude multiéchelle du transport de masse dans les bioélectrodes poreuses par microscopie confocale *operando* et modélisation numérique / Multiscale investigation of mass transport in porous bioelectrodes using confocal *operando* microscopy and numerical modeling

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Descriptif du projet

Redox enzymes are highly attractive for bioelectrochemical devices, such as biosensors and biofuel cells, because of their exceptional specificity and high catalytic turnover at low overpotentials [1]. However, their long-term performance remains limited by the sensitivity of these proteins to their local microenvironment. During high-rate catalysis, enzymatic reactions, often coupled to proton transfer, can significantly alter the local pH near the electrode surface. Because enzymes operate efficiently only within a narrow pH window, such local variations may decrease activity or even cause irreversible denaturation. While studies on planar microelectrodes have begun to characterize these effects, extending this understanding to porous bioelectrodes is essential for developing applications.

The main goal of this PhD project is to investigate mass transport and enzymatic electrocatalysis in porous electrode architectures through a multiscale experimental and modeling approach. Porous electrodes provide the high surface area required to achieve high current densities, but they also introduce complex transport limitations for substrates, products, and protons.

The project will map local concentration gradients, including proton and substrate distributions, within the three-dimensional structure of porous bioelectrodes under operando conditions, and will develop multiscale numerical models in COMSOL Multiphysics that integrate pH-dependent enzyme kinetics with diffusion-reaction phenomena in complex geometries [2].

The work will combine electrochemistry, fluorescence microscopy, and finite-element modeling. Porous electrodes will be fabricated from carbon-based materials, such as carbon nanotubes or porous carbon, or from ITO, and modified with model enzymes such as bilirubin oxidase for O_2 reduction or hydrogenase for H_2 oxidation. Fluorescence confocal laser scanning microscopy (FCLSM) will be used to visualize three-dimensional local pH profiles [3]. This technique is particularly well suited to optically transparent porous structures, such as transparent conducting oxides, and offers high spatial resolution. Three-dimensional multiscale models will then be developed in COMSOL to simulate bioelectrode behavior.

This research will provide a comprehensive understanding of microenvironment effects on bioelectrocatalysis. By validating COMSOL models against operando three-dimensional microscopy data, the project will establish a predictive framework for designing porous bioelectrodes and ultimately guide the development of more stable and efficient bioelectrochemical energy conversion and sensing systems.

Références Bibliographiques

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