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Titre de la thèse :

Electrochemistry and Spectroscopies in operando for reaction monitoring in molecular catalysis. Application to CO2 reduction and O2 activation.

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The REACTE group at LEM has made recent pioneering advances in the development of spectroelectrochemical cells for molecular catalysts in collaboration with beam scientists at SOLEIL, leading to a unique set-up for in operando studies. Based on these results, the present project aims at intensifying the use of spectroscopic (XAS, IR, MS) and electrochemical tools to perform in depth mechanistic studies during the electrocatalytic reduction of CO2 and/or O2 with transition metal molecular complexes (mainly Fe porphyrins). These in operando approaches will allow to determine the geometric and electronic structures of transient reaction intermediates and provide unprecedented mechanistic insights. This knowledge will help designing catalysts with improved efficiency and selectivity.

Mots clés : spectroscopies in operando; spectroelectrochemistry, XAS, IR; mass spectrometry; molecular electrocatalysis; activation of small molecules

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